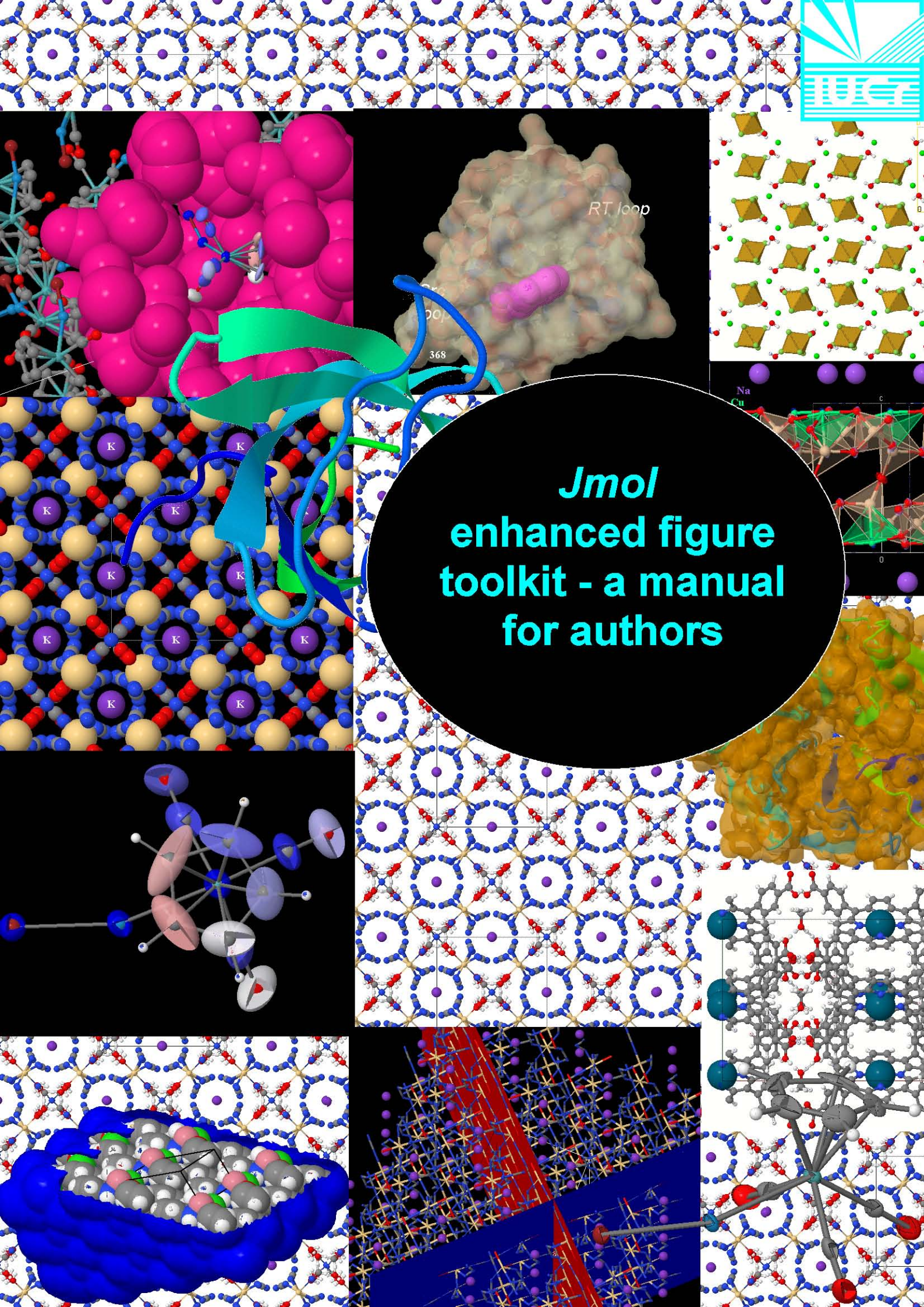
RT loop
368
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Jmol
enhanced figure toolkit - a manual for authors

Jmol enhanced figure toolkit – a manual for authors

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1. Introduction

Although interactive graphics programs for web content have been available for some time, and have been used in some very sophisticated online tutorials, they have not been widely used by academic journals. There are many reasons for this, including the impermanence of some of the programs, their requirements for particular supporting software or browsers, the difficulty with integrating online content into a conventional publishing workflow, or the difficulty in creating suitable high-quality content.

The IUCr journals now offer to authors a toolkit allowing the creation of enhanced figures for publication (McMahon & Hanson, 2008). The enhanced figures will be integral to the research articles in which they appear (*i.e.* they are not supplementary documents). They comprise two components: a static image, in TIFF and PNG formats, that appears in the PDF version of the article, or as a representation in browsers that do not support or enable Java and JavaScript; and a web page in which is embedded a full visualization program, *Jmol*, displaying the author's preferred view of a molecular or crystal structure (identical to the static image), but which may be manipulated by the reader of the journal. The enhanced figure web page may also contain buttons, checkboxes and radiobutton options helping the reader to interact with the displayed structure in specific ways designed by the author.

In this manual we explain how authors may use this toolkit to design value-added interactive graphics to illustrate and enhance the scientific message of their articles.

2. Why *Jmol*?

Jmol (http://www.jmol.org) is a richly-featured three-dimensional molecular visualization program that is widespread in the chemical, crystallographic and biomolecular communities. It is in many ways a descendant of *RasMol* and *Chime*, but it has significant abilities to represent features of particular interests to crystallographers that surpass those available in the earlier programs.

It has many features that have led to the IUCr journals adopting it as the engine for enhanced figures.

First, it is implemented in Java, a machine-independent language that is implemented as a virtual machine on all current operating systems of interest to most crystallographers. Java plugins are implemented in most web browsers, so that the end-user does not have to download the software – it is automatically loaded on demand the first time a browser visits a web page hosting a *Jmol* applet.

Second, it has a rich scripting language, so that external script files may be used to generate and drive particular views, renderings or animations. At the same time, it is easy for the end-user to manipulate the objects visualized with the mouse, keyboard and other computer peripherals.

Third, it is associated with a rich JavaScript library that allows the user to interact with the application through standard widgets found on a web page (buttons, checkboxes *etc.*) This makes it particularly easy to build a natural user interface to an enhanced figure.

Fourth, it has a very clean mechanism for exporting the current graphics state. If this exported state is imported into another instance of the applet, the exact same view will be regenerated. This is essential for an application that allows authors to edit a *Jmol* visualization on their own computers, taking advantage of their local processor power, graphics card capabilities *etc.*, but then to transmit what they have done back to the journals server, allowing it to create the static view and also to download the interactive representations to the journal readers.

Finally, it is an open-source project that is currently extremely well supported by active, talented and enthusiastic developers. At the same time, it is mindful of the need to maintain long-term compatibility with older programs and with older versions of the same program. These are features which are essential if we are to consider it as the basis for storing parts of the long-term record of scientific research.

3. When to use an enhanced figure

In general, the same principle should be followed as when creating normal figures: the author wishes to demonstrate to the reader something of scientific importance that is best shown in a visual way. Where all the important information can be seen in a static figure, that may still be the best way to present it.

However, an advantage that *Jmol* offers over a static view is that the reader may interact with the molecular structure, rotating it, viewing it from any angle, highlighting regions of particular interest, hiding those that clutter the view, measuring arbitrary distances and angles between atoms, *etc.*

If you are reporting a simple molecular or crystal structure, with no deviation from canonical bond lengths or geometries, you may feel that there is no real benefit to the reader in having access to an enhanced figure. (Remember that the online editions of the IUCr journals already provide a three-dimensional visualization using *Jmol* of every structure. The visualizations are accessible from the contents pages to non-subscribers, or from within the HTML edition of the articles by following the 'supplementary files' link.)

However, if your structure is complex in shape, or packs in ways that are difficult to represent clearly in a two-dimensional projection, then you may find it convenient and easy to prepare a simple enhanced figure that demonstrates these features, with little investment of time on your part.

As you become more experienced with the use of the enhanced figure toolkit, you will find it increasingly easy to add

scripts to the enhanced figure, which will provide the reader with different views of the structure, or with animations that demonstrate particular features of the structure and its properties.

The toolkit is designed to make it easy to create enhanced figures, and to include them as part of a submitted article. It integrates fully with the submission and review system operated by the IUCr journals, so that Co-editors and referees can see the enhanced figure and assess its worth to the article. Of course, this means that you must be willing to respond to reviewers' comments regarding the enhanced figure, and be prepared to make appropriate revisions if requested to do so.

4. How to submit an enhanced figure

Before you submit your article, you may use the toolkit described in this manual to create an enhanced figure in a form that will be compatible with the journals' production workflow.

4.1. 'Conventional' submissions

For most of the IUCr journals, you will submit a single file containing your article and all its tables, figures, supplementary information *etc.* The submission system will be revised in due course, so that you may upload individual source files for figures *etc.* at this stage. However, for the moment you will first prepare your enhanced figure, then provide a static version of it within your submitted article, along with a link to the online version.

The stages in this procedure are as follows.

1. Upload the Crystallographic Information File (CIF) containing structural data for the structure (or structures) you wish to illustrate. This is done through the upload page shown in Fig. 4 and discussed in more detail in the introductory tutorial.

2. Use the features of the toolkit to create the main illustration that will appear as the static figure in PDF versions of the journal. This figure will be made available to you as a static image in TIFF format.

3. If desired, make additional edits to create other custom views that the reader of the online edition will be able to access. The tutorials in this manual will explain the many options available to you.

4. When writing your article, include the TIFF of the static image to represent the main view of the figure. Provide a figure caption and discuss the information in this figure as you would for any other figure. Also supply alongside this figure the URL of the enhanced version, so that the Co-editor and referees may see the figure online. This URL will have been supplied to you when you first created the enhanced figure.

5. If any revisions to the enhanced figure are requested by the Co-editor, you may make further edits and notify the Co-editor when you have done so.

6. When your article is accepted for publication, you will proceed to the stage where individual source files (article body, figures, structure factors *etc.*) must be uploaded. At this point, you need simply paste into the upload page the URL of your enhanced figure, and it will be transferred to the journal production system (Figs 1, 2).

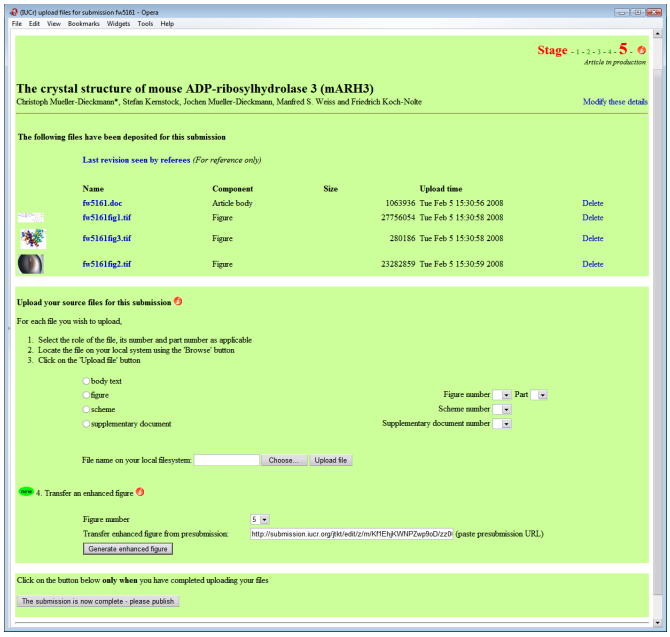

Figure 1
Transferring an enhanced figure to the submission system once an article has been accepted.

7. When your article is published, the static version of the figure will appear in the PDF or hard-copy editions; it will also be seen in web browsers that cannot or do not show active content. For all other readers, the enhanced figure will appear in their browsers as an interactive applet, complete with the additional scripts that you have provided and that the reader may activate by clicking on buttons or checkboxes.

4.2. Submission of structure reports

Acta Crystallographica Section C publishes high-quality studies of crystal and molecular structures, and *Acta Crystallographica Section E* publishes short reports of crystal structure determinations. In both journals, initial submission of the article is by means of a CIF that contains all the structural data for publication, along with the text of the article.

For these journals, it is possible to proceed as before, *i.e.* to create an enhanced figure before submission, and subsequently transfer it to the submission system. This can be done during

Figure 2
Once transferred, the enhanced figure is treated like any other.

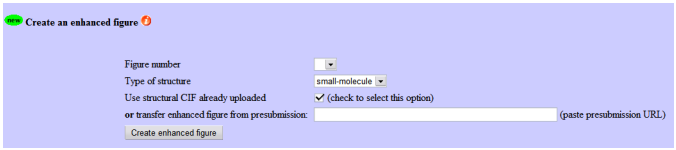

Figure 3
For structural papers, the enhanced figure may be created within the submission system once the CIF has been uploaded.

the early stages of submission, since these journals require you to upload all the source files before the material is assigned to a Co-editor.

However, for these journals it is also possible to create the enhanced figure within the submission system itself, once the CIF has been uploaded (Fig. 3). Indeed, for these journals this may be the best way to proceed, since the enhanced figure is guaranteed to be associated with the data set that forms the essence of the article.

5. An introductory tutorial

5.1. Upload structural data

An author wishing to prepare an enhanced figure before submitting an article comes to the start page, shown in Fig. 4.

It is important to enter an email address to which a receipt message will be sent. This message contains the URL that you will need to make future edits to the figure (each figure is given a unique and unguessable identifier). The message will also contain a second URL that should be cited within the article that you submit. This second URL will allow the Co-editor or referees to view your enhanced figure, but not to edit it.

If you wish, you may also supply a short label or tag that will appear in the subject line of the automatically generated email response. This can be helpful in identifying a particular figure if you plan to prepare several simultaneously.

Specify the type of structure you are illustrating – inorganic, small-molecule (this includes organic and metal-organic compounds and complexes), or biological macromolecular (proteins, nucleic acids *etc.*). This will set certain default values and styles appropriate to the type of structure you wish to illustrate, and will also select different editing palettes tailored to the requirements of that type.

Normally you will be uploading a CIF from your own computer to illustrate some new structure. You may specify the location of that CIF on your filesystem (using the 'Choose' button to browse the contents of your computer if needed).

Sometimes, however, you may wish to illustrate some aspect of a structure that has already been published or deposited in a structural database. If you know the reference code of such a structure in a public CIF archive (*e.g.* the Protein Data Bank or **Crystallography Journals Online**), you may enter the code on this page. At this time, 4-character alphanumeric codes (*e.g.* 1cro) are assumed to be protein structures deposited in the PDB; six-character codes of the form *aannnn* (where *a* is some alphabetic character, *n* a numeric one) are assumed to be structures published in IUCr journals.

If the CIF you are uploading contains several data blocks, by default the toolkit will load the first block containing structural data. You may select a different data block by specifying its numerical position within the CIF (do not count any blocks, such as those containing the text of an article, that do not contain structural data).

The special value 'all' will cause the toolkit to superimpose all models in the same visualization space. Note that this is rarely useful for crystal structures with different unit cells, but may occasionally be useful for comparing near-homologous structures.

You will understand this tutorial better by working through the steps with a real example. Enter 'sk3182' in the 'External database code' field to retrieve from the IUCr archive the CIF for the structure that we are using (Schlueter *et al.*, 2008): poly[potassium [diaquapenta-μ2-dicyanamido-dicadmium(II)] dihydrate].

5.2. The user interface

Fig. 5 shows the result of uploading a CIF, in this case of an inorganic structure. The main parts of the edit window are identified for future reference.

At this stage, the first thing that you should do is to save the file that you have uploaded. (It is possible to begin editing the structure immediately, but it is best to save so that you receive the email message recording your edit URL, and so that the necessary permanent storage resources are set up on the IUCr server.)

In this introductory tutorial, you should always save using the left-hand 'Save' button (the one marked 'Primary save' in Fig. 5). This will save the current view in the visualization window as the initial view of your enhanced figure, and will create a static image of this view for publication in the PDF edition of the journal.

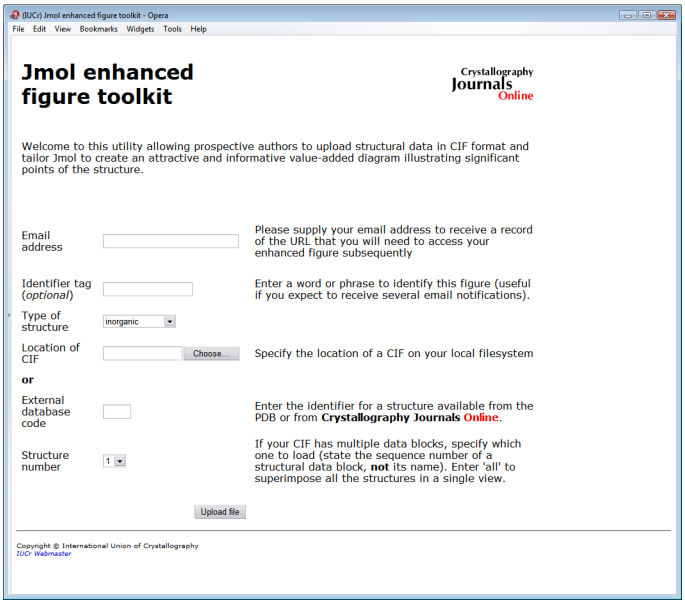

Figure 4
The start page for creating an enhanced figure.

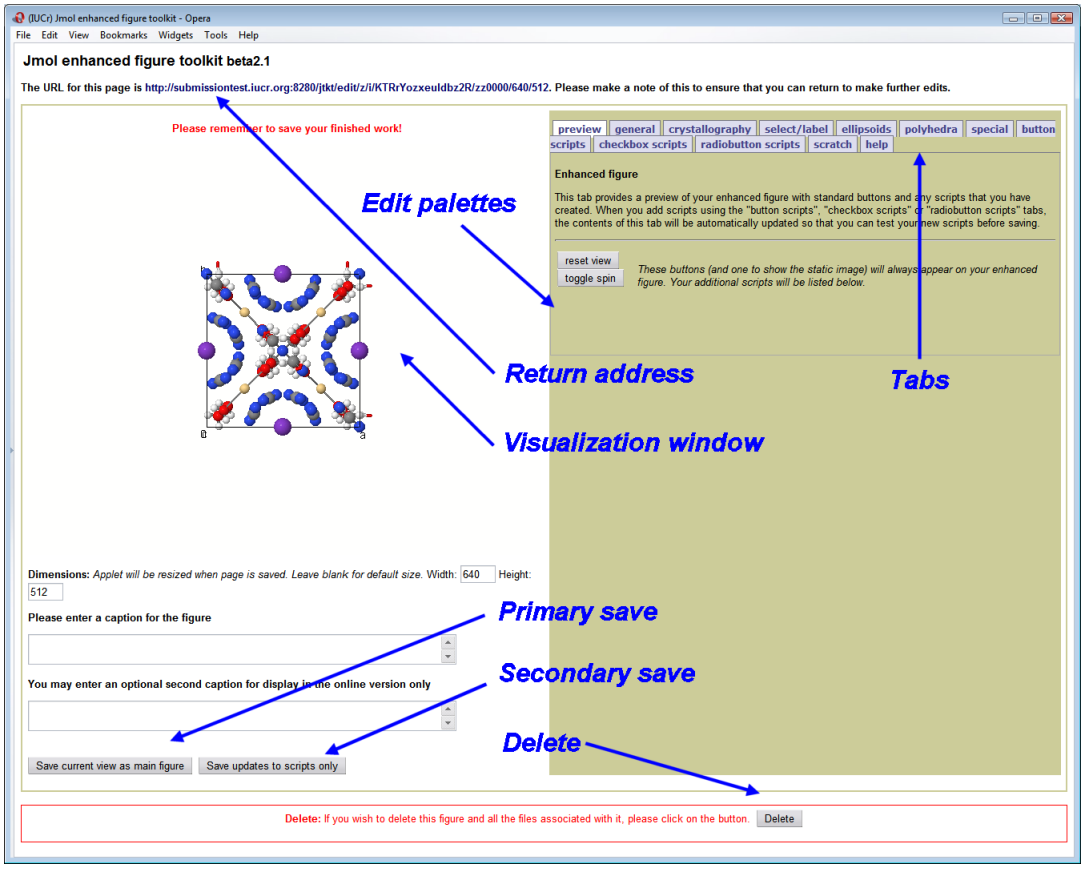

Figure 5
The main edit page of the *Jmol* toolkit immediately after uploading a CIF. The major areas of the page are identified.

Fig. 6 shows the result of saving at this point. The top of the page summarises the information that you need to use the figure in your article submission.

The bottom of the page shows the enhanced figure that you have created. It contains a *Jmol* applet showing a default view of your structure. This is a fully interactive applet – a reader may move it around with the mouse, and access all the functionality of the *Jmol* applet by right-clicking within the applet.

On the right-hand side of the figure, a number of standard buttons have been placed for the reader. From the bottom up, they are: 'toggle spin', which starts or stops the structure rotating about a vertical axis in the plane of the screen; 'reset view' which returns to the starting view; and 'static view', which replaces the applet by the static image that will be used in the PDF edition of the journal.

You should click on the 'static view' button to check that the static image has indeed rendered correctly.

5.3. A simple edit

Now click on the 'Return to editor' button to return to the main edit page (Fig. 5). Alternatively, if you were to shut down your browser, you could return at any later stage to the editor using the URL that was mailed to you in the receipt message. It is also displayed as the 'Return address' on the edit page.

We shall create a packing diagram of this structure to demonstrate its beautiful symmetry in an extended crystal lattice.

Click on the **crystallography** tab in the right-hand panel to display a number of options allowing you to display particular features of the crystallographic symmetry. Fig. 7 shows the initial settings of the controls available to you on this tab.

One thing that you should be aware of is that the checkboxes, menus and radiobuttons control JavaScript functions that communicate commands to the Java applet. Using these, you will be able to change the appearance of the structure displayed by *Jmol*. However, there are other ways to change the graphics state of the object in the applet (some of these will be discussed in later tutorials). If you change some aspect of the display by one of these other means, the checkboxes *etc.* in the edit palette will *not* necessarily reflect those changes. That is, the checks or other selection marks against the items on these palettes are not guaranteed to reflect the current graphics state.

This is an inherent shortcoming of the loose coupling between *Jmol*, which is a Java applet, and the JavaScript commands which your browser can implement. You should find with a little practice that this does not greatly reduce the usability of the toolkit.

However, you should bear in mind that the same shortcoming will be present in the interactive figures that you are planning to create, and you should therefore take care to minimise the

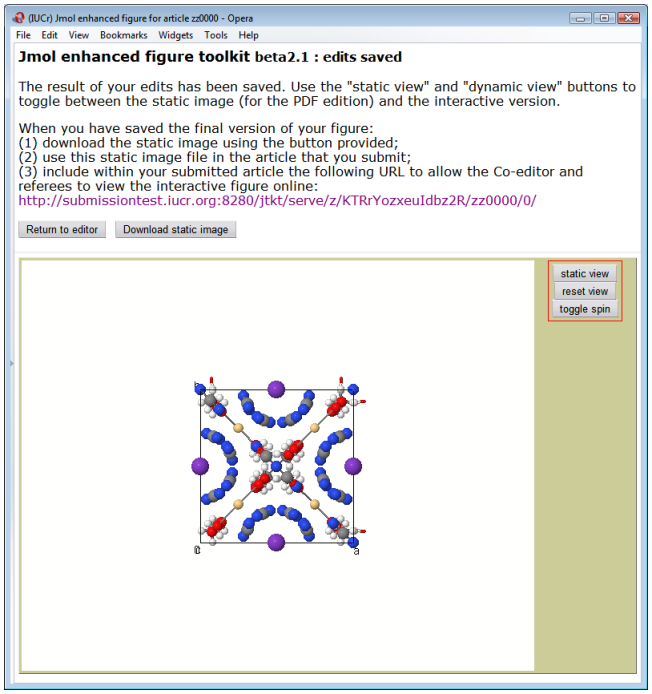

Figure 6
The result of an initial save of the enhanced figure.

chances for inconsistency in the functions that you provide to the reader. Later tutorials will revisit this consideration.

Go now to the pull-down menu under the heading 'Cell packing' and select the option '3 × 3 × 1 unit cells'. The display in the *Jmol* window immediately changes to show the crystal packing down the **c** axis (Fig. 8).

You can appreciate the pattern better by zooming out. If you have a mouse with a scroll wheel, click in the applet window and zoom out using the wheel, until you have a view that just fits into the image area. Alternatively, hold down the SHIFT key and the left mouse button and move the mouse vertically up or down to zoom.

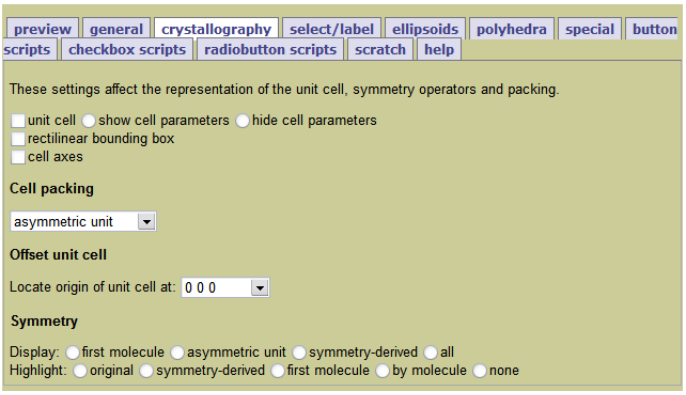

Figure 7
The options for displaying different aspects of crystallographic symmetry.

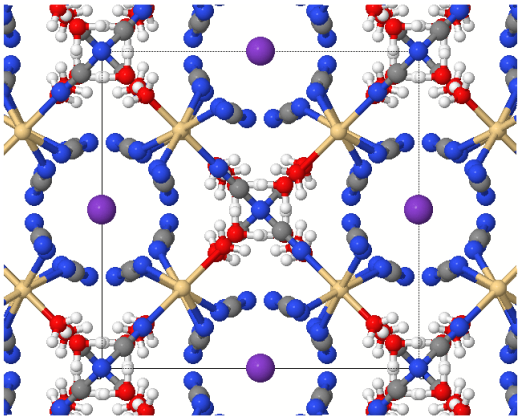

Figure 8
Crystal packing generated from a pull-down menu on the **crystallography** edit tab.

Now you may add a figure caption. Two boxes are provided for captions. Use the upper one for any comment that applies solely to the current view (*i.e.* to the image that readers of both PDF and HTML versions of the article will see). In this example we add a second caption ('the interpenetrating layers are best seen in an oblique view') that invites the reader to explore the packing by moving the structure around.

Save this, using the 'Primary save' button as before, and you have created your first enhanced figure for publication (Fig. 9)!

5.4. Good housekeeping

If you decide not to submit the figure for publication, it is only polite to remove it and the associated storage from the IUCr server, by clicking on the 'Delete' button at the foot of the edit window (Fig. 5).

The IUCr server routinely deletes files that have not been accessed for a certain period of time (currently three months). This should provide adequate time to prepare and submit an article. However, if review of the article is taking longer than this, you should return to the figure and refresh the files (a simple save will indicate to the server that the figure is still active).

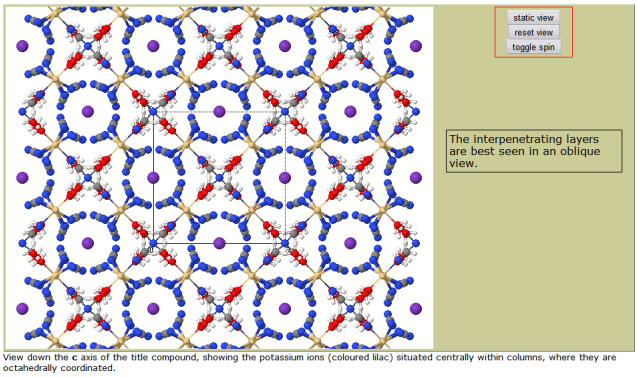

Figure 9
Enhanced figure, showing main caption (applicable to static and interactive views) and secondary caption (relevant only to the interactive view).

6. Tutorial 2: an inorganic crystal lattice

6.1. Lesson 1: using the standard palette functions

In this second tutorial, we revisit the inorganic structure sk3182 and use it to develop a number of new skills, from the perspective of an author who is not familiar with *Jmol*.

Begin again with Fig. 5, representing a structure that has just been uploaded. The first option that you see, just below the visualization window, allows you to change the size of the applet. The default size (640 × 512 pixels) is a standard size used in the online journals, and should be used unless there is a good reason not to. Suppose in this case that the Co-editor agrees that a square format figure better displays the symmetry down the **c** axis of the tetragonal lattice, and so change the height to 640 pixels. (In general, changes to the width should *only* be made with the agreement of the Co-editor.) You should now save the figure before doing anything else. (Again, use the primary save button at this stage.)

Now consider the tabs allowing you to switch between different editing palettes. The tabs that are present (and their contents) depend on the type of structure. For inorganic structures, as in this example, the tabs that provide particular *Jmol* functions are entitled

preview: allows testing of any scripts used in the enhanced figure

general: for overall aspects of style or representation

crystallography: for illustrating aspects of the structure arising from crystallographic symmetry

select/label: for selecting and labelling individual atoms or groups of atoms

ellipsoids: for drawing atomic displacement ellipsoids

polyhedra: for drawing coordination polyhedra

special: for some special effects

For biological macromolecules, a **structure** tab allowing different stylised representations of secondary structure replaces the **polyhedra** tab; for small-molecule structures both of these are absent.

In general it is useful to work along the tabs from left to right, but you may always switch between them at any time, as appropriate.

For this example, start with the **general** tab. Select a black background to show the differently coloured atoms with higher contrast; then choose 'ionic radii' in the drop-down menu of atom radii.

Now move on to the **crystallography** tab. In the first tutorial, we selected '3 × 3 × 1' in the 'Cell packing' menu, which nicely demonstrates the symmetrical packing in the **ab** plane. However, in this crystal structure the novel feature is the interpenetrating sheets *along* the **c** axis, which are difficult to visualize in a single unit-cell depth. Therefore select 3 × 3 × 3 as the cell-packing option, to allow the reader to appreciate the variation with depth as the crystal structure is viewed from different angles. Zoom out (using the mouse scroll wheel, or SHIFT + left mouse button) until the image just fills the applet.

Notice that the atom radii have reverted to their default sizes. This is because the commands to generate the space-filling diagram override the existing specifications for atom sizes. You can fix this by returning to the **general** tab and re-selecting the required option in the 'atom radii' menu.

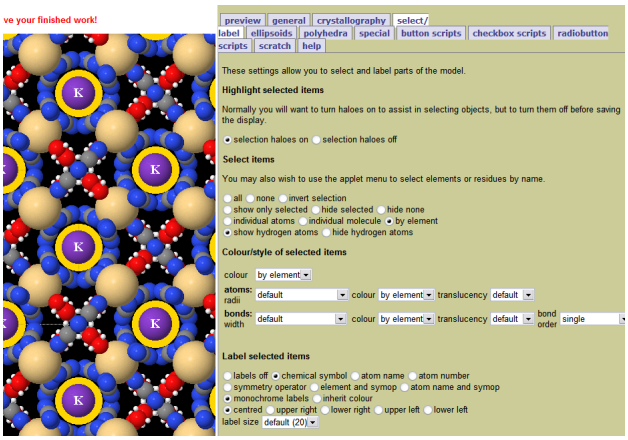

Figure 10
Using the **select/label** tab to select K ions (in lilac, and surrounded by yellow selection haloes).

Now label the K ions, which have been singled out for comment in the caption. Go to the **select/label** tab. *Jmol* provides a very rich set of scripting commands to select individual atoms or groups of atoms. The buttons on this page provide access to many of these commands, but their interactions with each other are not always intuitive. The first thing that you should do, therefore, is activate the option 'selection haloes on'. This will draw a translucent yellow sphere around each atom that has been selected - initially, all of them. Now click 'none' in the main set of buttons in the 'Select items' section, and then 'by element' to restrict the selection to an individual element. Now, when you click on a K ion, all other potassiums in the structure will be simultaneously selected (Fig. 10).

Now label the K ions using the set of buttons grouped under 'Label selected items'. Select the options 'chemical symbol', 'white labels', 'centred', and leave the label size at the default value.

Now turn 'selection haloes off', so that they are not rendered in the enhanced figure. You should also click 'all' under the 'Select items' heading. This will not now have any visible effect, but will ensure that the *Jmol* applet presented to the reader will have the default 'select all' state active. If you do not do this, a reader who has experience of *Jmol* will find that the applet does not behave as expected.

Finally, select the option 'hide hydrogen atoms' on this tab, to remove visual clutter, and save the result as your new enhanced figure (Fig. 11).

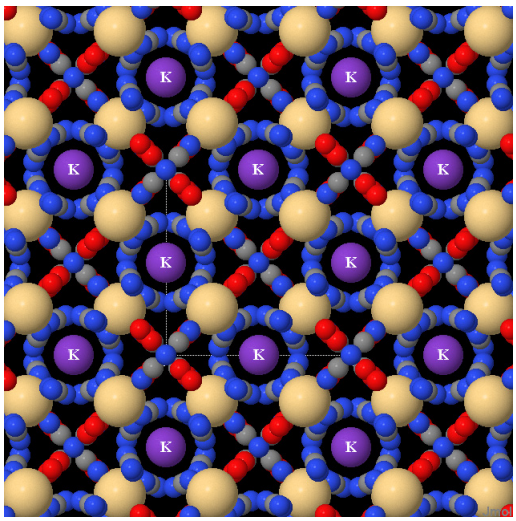

Figure 11
The initial view of the enhanced figure created in Tutorial 2.

6.2. Lesson 2: adding features to the enhanced image page

In this lesson you will provide options to the reader for viewing the crystal packing from different directions.

When you move the current view away from its orientation down the **c** axis, the large atoms clutter the view. You can obtain a better impression of the packing from different viewpoints by reverting to a simple stick representation, where only the bonds are shown. On the **general** tab therefore use the 'overall style' menu to select 'sticks'. The K ions are not shown as bonded, and so disappear from view (although their labels are still visible). You can address this by going to the **select/label** tab; select 'none' to ensure that any existing selections are cleared (again you may find it useful to switch selection haloes on while you perform these operations); select 'by element' and then click on a K ion; in the area headed 'Colour/style of selected items' choose an atomic radii value of '20% van der Waals'; select 'labels off' (you may need to select another option first); and finally select 'all' and switch selection haloes off.

All this is tedious to describe, but comes naturally with a few moments practice. The result is a more schematic view of the crystal packing (Fig. 12).

Now go to the **button scripts** tab (Fig. 13). This allows you to input up to four *Jmol* scripts, each of which will be associated with a button on the enhanced image page that will run this script when selected by the reader.

For the moment, we suppose that you do not know any commands in the *Jmol* scripting language. Nevertheless, you can still make use of this page. Click on the topmost button marked 'import view'. This will copy into the adjacent field the entire graphics state of the image currently in the visualization window. You should write a caption to describe this view in the field provided – something like 'Schematic view of the crystal packing down the c axis.'

You can see the effect this has had by switching to the **preview** tab (Fig. 14). Now, in addition to the standard buttons for recovering the initial view and toggling the spin state, there is a new button, labelled '(a)', that links to the script you have just created. Use your mouse to move the crystal packing diagram around, then click on this new button. You will see that it returns the view to the one that you selected.

Now save what you have done. This time click on the 'Secondary save' button, the one marked 'Save updates to scripts only'. Do **not** select the button marked 'Save current view as main figure': if you do, then the view currently in the visualization window will overwrite the view that you have previously saved. You will now see the new button also on the enhanced figure page.

Now return to the editor, and repeat the procedure outlined above to create the schematic bonds-only view of the packing.

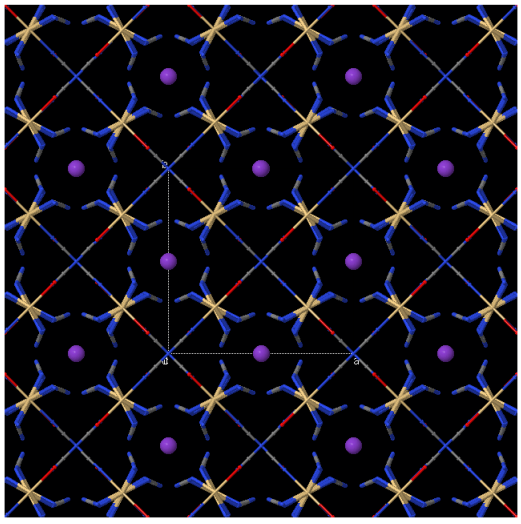

Figure 12
A simpler view of the crystal packing that is provided as an optional view.

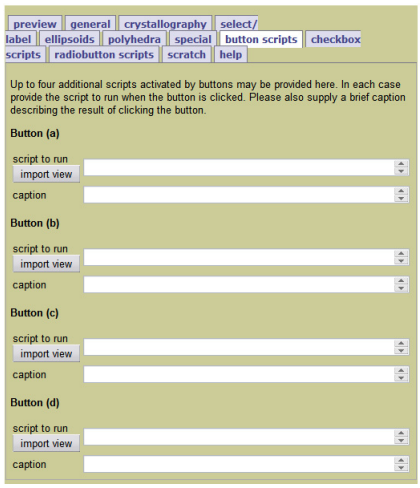

Figure 13
The **button scripts** edit tab.

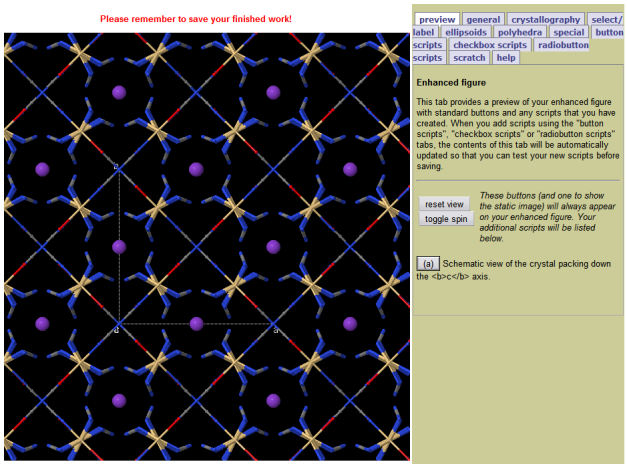

Figure 14
Using the **preview** edit tab to test the effect of the new script.

(There are other ways to retrieve this new view that we shall describe in later tutorials. At the moment, however, go through the exercise again, for practice. On the **general** tab, select the Orientation: 'right: bc plane at back, a axis outward'. The packing diagram should rotate to that orientation. You may need to zoom in to re-fit it to the full applet window.

Go to the **button scripts** tab and click on the *second* button that says 'import view'. This will paste the current graphics state into the second scripts window. Add an appropriate caption below this.

If you really need the practice, you can repeat the entire cycle, but instead just go to the **general** tab, select the 'top' orientation, resize the image, return to the **button scripts** tab, import this view, and add an appropriate caption.

Finally, manipulate the model to find an oblique view where interesting motifs of the packing are apparent, and save this in

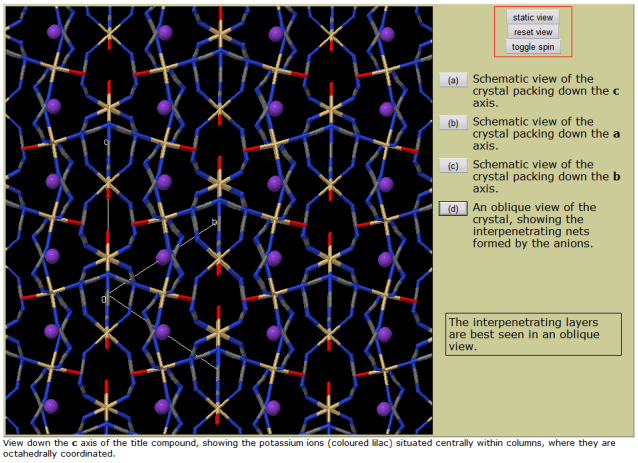

Figure 15
The new enhanced figure with options for the reader to access different selected views. In this figure, option (d) has been chosen, and the reader sees the author's preferred view of the interpenetrating nets. Of course, the reader may now manipulate the viewpoint to clarify (or further obscure!) the details of the packing.

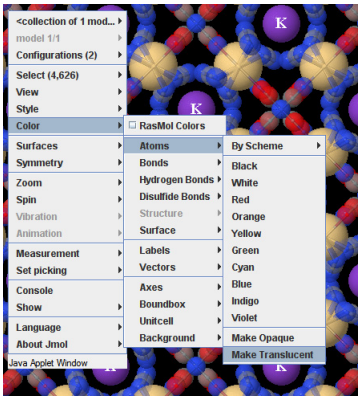

Figure 16
The *Jmol* menu allows you to use many of the same editing features available elsewhere in the toolkit.

the slot for the fourth script. Now save what you have done (again using the 'Secondary save' button) to find that you have created the result shown in Fig. 15.

6.3. Lesson 3: using the Jmol menu

If you have used *Jmol* before, you will be aware that you can access many of the features of the program through a pop-up menu that you activate by right-clicking in the applet window (Fig. 16). You may use this menu to change the appearance of the model in the visualization window. Many of the menu options are implemented within the different editing palettes within the toolkit, and you may use the *Jmol* menu or the palettes interchangeably. Sometimes it is simply more convenient to work completely within the area of the applet; at other times the edit palettes may provide easier access to the options you want to use.

An interesting case is shown in Fig. 17. *Jmol* creates its menus dynamically, and can change certain features according to the nature of the current model. In our example structure, there is some positional disorder associated with an oxygen atom. This is represented in the CIF by assigning the disordered atom to two alternative locations. *Jmol* recognises these as distinct configurations. By default, both are visualized; but the *Jmol* menu allows you to select one or the other. In Fig. 17 we show how to select one of the alternatives in order to reduce the visual clutter of the disordered site.

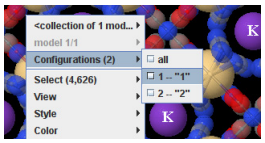

Figure 17
Sometimes the *Jmol* menu offers the only easy way to modify context-sensitive visualizations of the structure.

6.4. Lesson 4: introduction to Jmol scripting

In Lesson 2, you added new scripts to the enhanced figure page using the 'import view' buttons. This imports a complex *Jmol* script describing fully the current graphics state. It has the advantage that you are able to generate complex views using the toolkit interface without needing to know anything of the *Jmol* scripting language. On the other hand, it is quite a heavyweight approach, since it generates many commands, and reproduces a very specific view. You may wish to provide the reader with options to perform various operations, and for this it's helpful to know at least a few basic *Jmol* commands. Many of these are very simple, and we provide a summary of some particularly useful ones in Appendix A.

The scripts that you have already added to the enhanced figure page are run when the reader clicks on a button. A button interface is perhaps the most natural for a script that will run once to provide a fully controlled, predictable effect – an animation, or a specified view with specific styles of atoms, bonds *etc*.

To provide additional options to the reader, you might consider 'checkboxes' or 'radio buttons'. In general, checkboxes should be used to provide functions that act independently of each other, and so are additive. Normally, the action of a checkbox is reversed when the box is cleared. Radio buttons are used to select among mutually exclusive options. The *Jmol* toolkit provides for up to four checkbox scripts, and one or two groups of radio buttons, each with up to six options.

Begin with a simple example (Fig. 18). Supply a script to run when the checkbox is selected ('stereo on'); a complementary one to run when the checkbox is unselected ('stereo off'); and a very brief caption to explain to the reader the purpose of the box. We recommend finishing each *Jmol* script command with a semicolon as a matter of good practice, although the toolkit's save procedure should normalize these if you forget to do so. You can switch to the **preview** tab to see how the new option for stereo rendering has been added to the output page.

Now return to the editor, and add a set of mutually exclusive options. As an example, we show in Fig. 19 the commands to render the current view in different styles – space-filling, ionic radii, ball-and-stick, or stick.

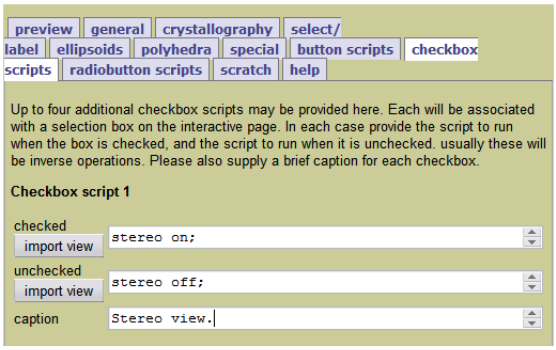

Figure 18
A simple checkbox script. Up to three additional such scripts may be added.

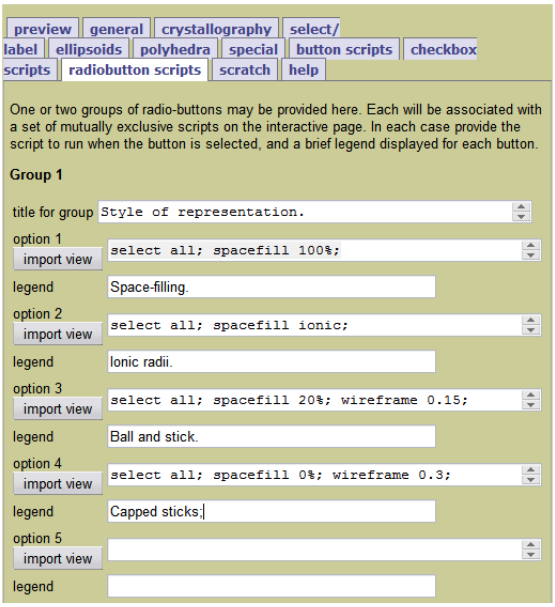

Figure 19
A group of mutually exclusive scripts implemented as a 'radio-button group'. Each group may contain up to six options. One or two groups may be created. The caption describing the function of the group as a whole is optional, but may be useful for the reader.

Fig, 20 shows the result obtained by a reader, who has selected the button option (d) to obtain the oblique view of the cell packing, then rendered the view in stereo (zooming out to get a better impression of the three-dimensional effect), and selected a ball-and-stick representation.

6.5. Lesson 5: becoming a power user

In the previous lesson you used some raw *Jmol* script commands. To get the most out of this application, there is no substitute for learning the *Jmol* scripting language, which is very well

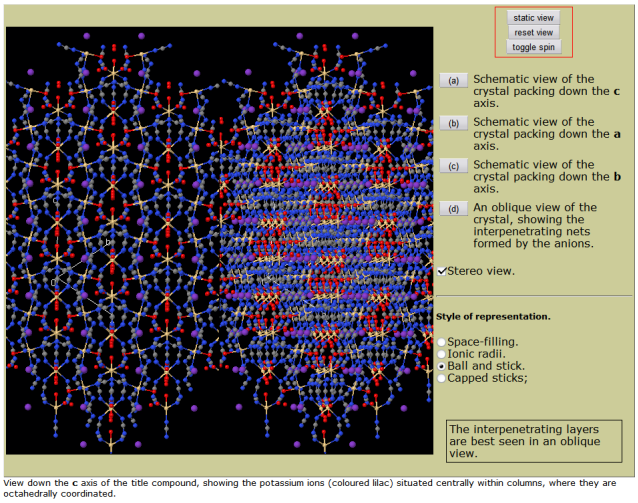

Figure 20
The interactive figure with many user-selectable options.

documented on the *Jmol* web site. However, it is a large and often complex language, and considerable investment of effort will be needed to become an expert.

The toolkit provides some utilities that will help the novice *Jmol* scripter to build up knowledge and experience of this language, and in lesson illustrates some of these features.

6.5.1. The Jmol console In Lesson 4 we introduced the idea that simple *Jmol* scripts, such as those sitting behind many of the buttons in the toolkit editing palettes, could usefully be copied as scripts for the use of the reader. Here we show how to use the *Jmol* console to discover from the toolkit what those commands actually are.

The console is a window that allows communication between the user and the *Jmol* application. It can be launched from the *Jmol* pop-up menu; in Fig.16 the 'Console' command may be seen near the bottom of the leftmost menu panel.

The console window has two main panes. The lower is an interactive shell, into which the user may type (or paste) commands for *Jmol* to execute. The upper pane returns information from the applet. The buttons along the bottom control aspects of the communication.

In the example of Fig. 21, you can set a stereo-view representation using a menu on the **general** edit tab. This splits the molecular view into two halves; the view in the right half is rotated by 5°, a typical displacement for comfortable cross-eyed stereoscopic visualization. Now bring up the console from the *Jmol* menu, and select the 'History' button at the bottom of the console. The upper window pane is filled with the commands that *Jmol* has most recently executed. Most of these represent the detailed setting of the graphics state during the loading process. At the bottom of the pane, however, you can see 'console', representing the command to bring up the console window, followed by 'stereo -5'. This last is the command to create a stereo pair offset differing by a 5° rotation. Select the 'wall-eyed stereo' option from the edit palette, click again on 'History', and you will see the command 'stereo 5' – clearly representing a 5° rotation in the opposite sense. Immediately you have has learned how to specify side-by-side stereo views to *Jmol*, and indeed how to change the angle of rotation to some value other than the default.

If you want to test the effect, say, of a 10° rotation, simply type in the lower pane of the console window the command 'stereo -10' and click on the 'Execute' button; the result of the command is immediately shown in the visualization window.

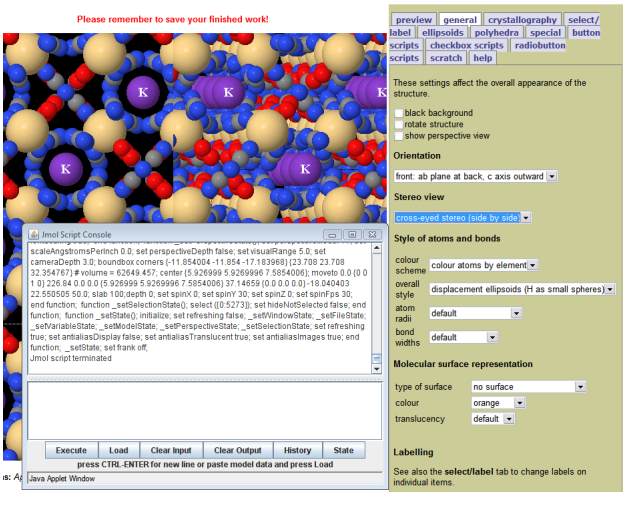

Figure 21
The contents of the *Jmol* window showing the application history after the user has selected 'cross-eyed stereo' in the **general** edit palette (right of screen).

6.5.2. Experimenting in the Jmol scratch window The toolkit provides a workspace for experimenting with *Jmol* commands on the **scratch** tab. Note that anything you do here can be done with the *Jmol* console directly, by cutting and pasting or by interactive scripting. However, for some users this may be a more convenient interface.

You can use this scratch workspace to figure out a way of highlighting some of the crystal planes for special attention. As you explore the available palettes, you may come across the options on the **special** tab for slicing through the crystal along a number of planes. Fig. 22 shows an example of the crystal sliced along the (220) plane. It is not exactly what we want – we do not want the space-filling representation that the menu has forced upon us; we wish just to highlight a plane rather than cropping to it; and we may wish to emphasise some planes other than those available to us through the menu. However, it is a promising start.

From the console history, you can see that the last commands executed by the applet in creating this view were

```
load "" 444 666 1;spacefill 100%;slab on;
isosurface p1 hkl 1/2 1/2 0; isosurface off;
slab plane $p1;
```

Copy and paste these into the text field on the **scratch** tab (Fig. 23). By inspection, you might suppose that the first command reloads the structure, displaying a range of 27 unit cells (from the symmetry operator codes 444 to 666), and that the second is what

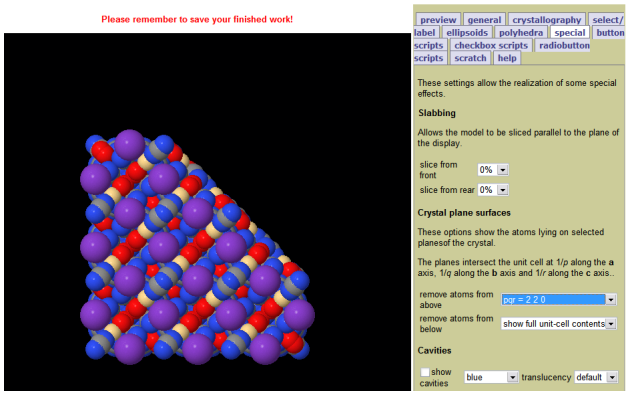

Figure 22
The toolkit is used to slice through a crystal plane.

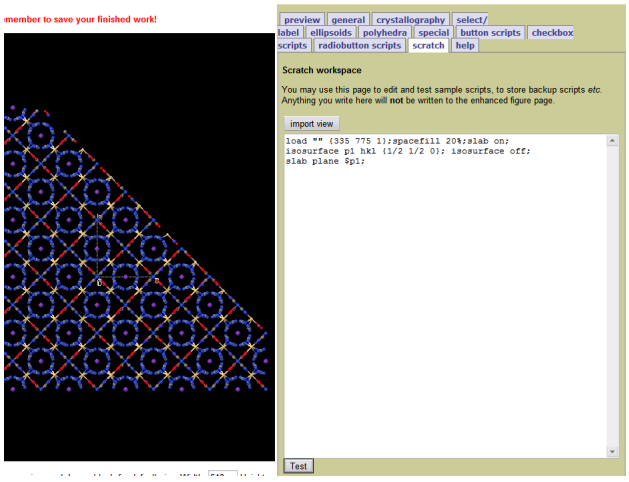

Figure 23
Modifying the view by testing new *Jmol* commands in the scratch workspace.

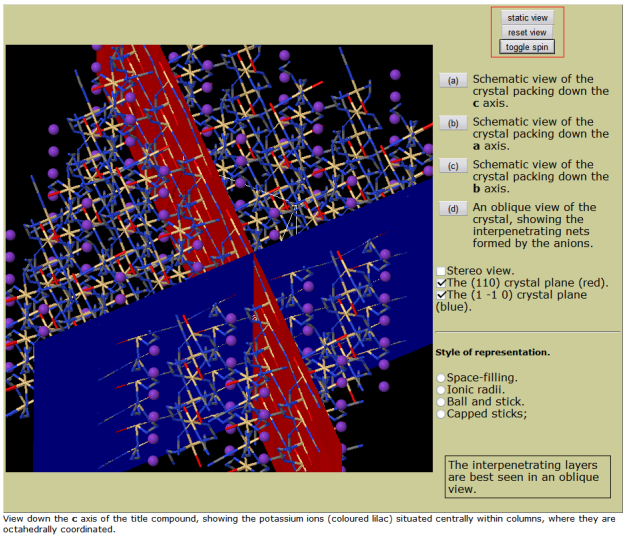

Figure 24
The final version of the enhanced figure. Two new checkbox scripts have been added, to highlight the (110) and (110) planes.

generates the spacefilling view. Test this hypothesis by changing the first line to

```
load "" 335 775 1;spacefill 20%;slab on;
```

and clicking on the 'Test' button below the scratch window. You will see that you now have a ball-and-stick representation, and that the portion of the crystal depicted shows 5×5 unit cells in the **ab** plane. By continuing to experiment in this way, you will find that the 'slab' commands are what determines how much of the structure is actually displayed. You can remove these. The 'isosurface' commands are used to specify the plane through a given set of *hkl* indices. If you remove the 'isosurface off' command, you will see that the first 'isosurface' command actually renders a plane. If you wish to provide the reader with a script that does not affect the existing atom/bond style or the amount of the crystal on display, you can indeed also remove the portions of this script that affect these parameters.

In the end, you will find that a script such as the following will simply display a plane described by a particular set of Miller indices (in this case 110):

```
isosurface p1 hkl 1 1 0; color isosurface red; show
$p1;
```

and the plane may be removed with the script

```
isosurface p1 delete;
```

These could conveniently be the complementary scripts written to determine the on/off events associated with a checkbox (Fig. 24).

Of course, one may need to consult the *Jmol* documentation and not rely solely on trial-and-error. Nevertheless, the scratch workspace allows you to test various scripting ideas without having to save the figure to see the effects of your changes.

When you have worked out a satisfactory script in the scratch workspace, you may copy and paste it from the scratch window into any of the other script entry boxes that the toolkit supports.

6.5.3. Other uses for the scratch window As with the other fields for *Jmol* scripts, the scratch window has an 'Import view' button allowing the complete graphics state of the image in the visualization window to be captured. This can be useful to capture an initial view that will be modified by subsequent additions or edits. The scratch window is designed to be large enough to allow a reasonable amount of interactive editing.

By contrast, the script fields on the other tabs are rather small – typically exposing only a line or two of text. This allows for several to be visible on the same page; it also encourages the use of short, one-line *Jmol* scripts, rather than unduly long or complex ones. On the other hand, if a large script has been stored in one of these fields that requires subsequent editing, the most convenient way might be to copy and paste it into the scratch window, manipulate it there (with the ability to make live tests on any changes you make); then finally paste the finished script back into its initial slot.

Note that the contents of the scratch window are retained when the enhanced figure is saved, although they do not find their way onto the final page created for the reader. This allows the scratch window to be used as a persistent store of specific scripts. In particular, it could be used to backup the main figure, in case you inadvertently overwrite it at a later stage by clicking on the wrong 'save' button.

7. Tutorial 3: a small metal-organic molecule

7.1. Molecular view with displacement ellipsoids

The 'standard' view of a small-molecule structure determined by X-ray crystallography is typically a minimum-overlap view of a single connected molecule, with atomic displacement tensors represented by real-space probability ellipsoids in the manner of the classic program *ORTEP* (Johnson, 1965). In this tutorial we demonstrate how to use *Jmol* to create such a view to the standard normally

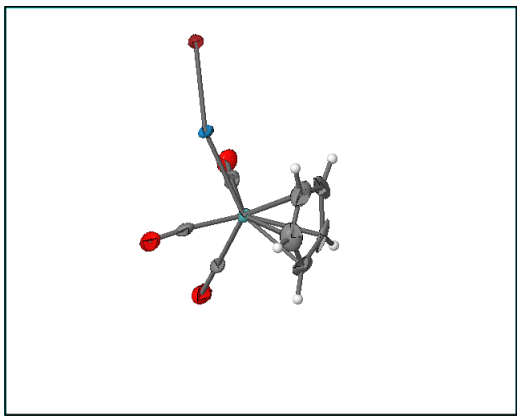

Figure 25
The on-load view of a small-molecule structure, showing 50% probability ellipsoids.

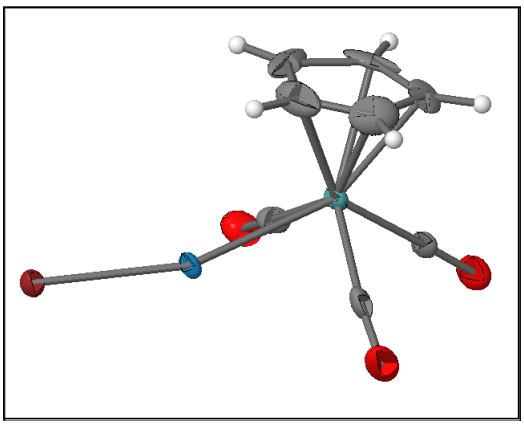

Figure 26
The molecule after repositioning to fill the visualization window.

required for ellipsoid plots by IUCr journals. For this example we use the bromido-1κ*Br*-tricarbonyl-2κ^3*C*-(2η^5-cyclopentadienyl)molybdenum(I)tungsten(I)(*W* – *Mo*) compound described by Onani *et al.* (2008). You may follow along with this tutorial by entering the code dn2343 in the toolkit start page (Fig. 4). Remember also to designate this as a *small-molecule* type of structure from the drop-down menu on that page.

Fig. 25 shows the initial view generated by *Jmol*. It displays the molecule oriented within the crystallographic unit cell viewed down the **c** axis, with **a** running to the right and **b** upwards. The view is centred on the *centroid* of the molecule. In this example, the default view is, by good fortune, not far from a minimum-overlap view, but it is not guaranteed to be so. In any case, you will wish to adjust the view for other reasons.

Begin by rotating the compound through 90° around the *z* axis, so that the pentacyclodienyl group sits to the upper right. Now zoom in so that the view almost fills the width of the visualization window. (The static figure that is generated for use in the PDF edition will be cropped of surrounding white space, so that filling the view helps to minimize the size difference in the online edition between static and dynamic views.) You should also translate the molecule so that it fits the visualization window most closely (lateral translations are performed in the most common configuration by holding down the CTRL key while dragging with the right mouse button). Fig. 26 shows the result.

Now begin to label the figure. Go to the **general** tab, select the 'atom name' option in the 'Labelling' section, and also select 'monochrome labels'. The result uses an appropriate typeface and font size for the static figure, but the default positioning of many of the labels is poor (Fig. 27). Much of the effort in producing an acceptable primary view of the enhanced figure lies in positioning the labels properly. While the edit palettes provide some tools to help with this, in many cases you will need also to enter explicit commands through the *Jmol* console.

Go to the **select/label** tab, and choose the 'lower right' option in the set of buttons headed 'Label selected items'. The result is already an improvement (Fig. 28).

Now it is necessary to select individual atoms or groups of atoms which will share the same label offset. It is helpful to toggle 'selection haloes on', which will highlight all the objects selected at any time. When you first do this, you will see that all the atoms are highlighted; so begin by clicking 'none' in the 'Select items' list. Now notice that the labels on all three oxygen atoms just touch their ellipsoids, and would benefit from a slightly greater offset. Click on the 'by element' button of the 'Select items' group, and then click on one of the oxygen atoms. You should find that all three are now highlighted. At this point you should bring up the *Jmol* console window (right-click in the applet, and choose 'Console' from the pop-up menu – see

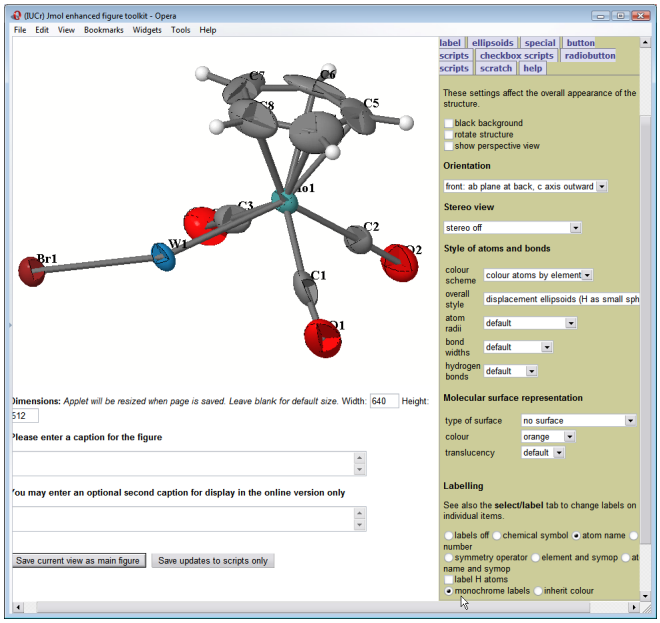

Figure 27
The default labelling options select the appropriate font and type size, but result in many labels that are poorly positioned.

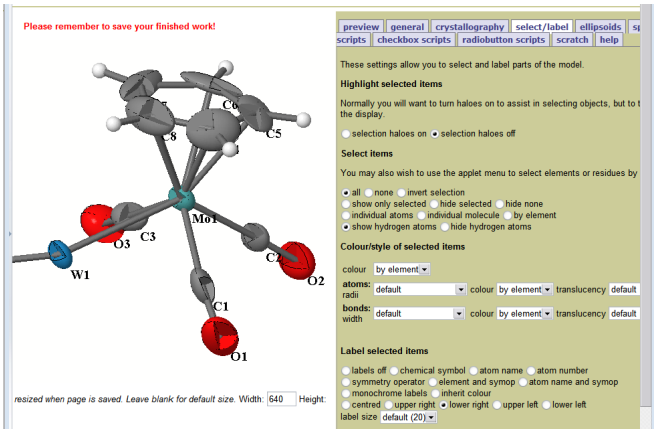

Figure 28
Placing the labels to the lower right of their corresponding atoms produces an immediate improvement.

also Fig. 16). If you click the 'History' button in the console window, you will see the command 'set labeloffset 12 -12' that was invoked when you selected the global 'lower right' option. Enter into the lower window of the console the command 'set labeloffset 14 -14'; you will find that the oxygen-atom labels move slightly, and are now correctly placed (Fig. 29).

Now you need to fine-tune the other labels. Ensure that you have no atoms currently selected, then click on the 'individual atoms' radiobutton. In this mode, clicking on an individual atom adds it to the currently selected set; clicking on it again removes it from the selection. The following selected sets and corresponding label positioning commands were used to obtain the finished view of Fig. 30:

Mo1, C6, C7	upper left
C2, C5	upper right
C8	lower left
C4	set labeloffset 36 -12
C1	set labeloffset 18 0

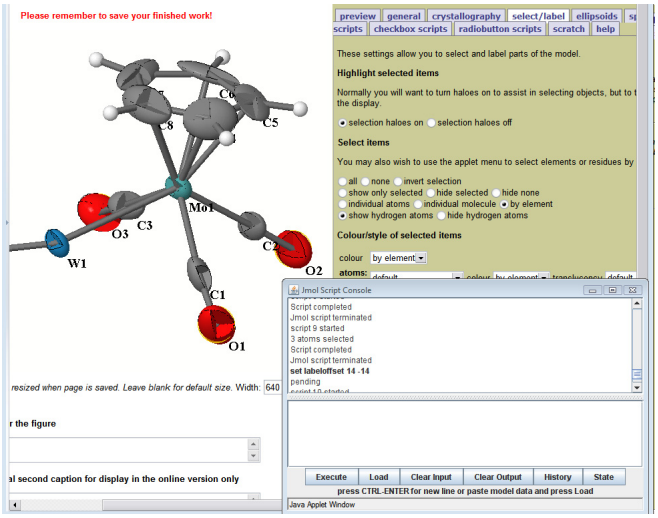

Figure 29
Using the *Jmol* console window to change the label offset for the current selection (here the three oxygen atoms).

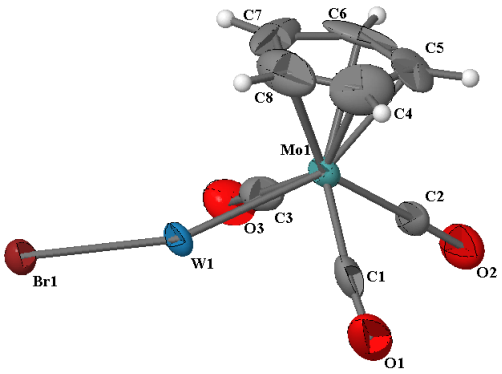

Figure 30
The final labelled view with offsets set on an individual basis.

Once you have finished these manipulations, you should ensure that all atoms are selected, then turn off selection haloes before saving the final result (Fig. 30).

7.2. Doing other things with ellipsoids

The default for displacement ellipsoids when a CIF is loaded into the toolkit is at probability 50%, solid with a cutout octant and with principal ellipses rendered. Although the principal ellipses are not always apparent at screen resolution, they are more obvious in the high-resolution static figure (Fig. 31).

Jmol also provides different styles of rendering, accessed through the options on the **ellipsoids** tab. These include solid ellipsoidal volumes and various simplified representations showing only midplanes, principal ellipses or principal axes. Although these are not generally suitable for the main view of the molecule, they can be helpful in different enhanced views, especially for large molecules or packing diagrams where the computational burden of rendering solid ellipsoidal volumes is high. There is also an option for displaying the wireframe outlines of the ellipsoids (or other solid objects) while the model is being manipulated. This can make it much easier and faster

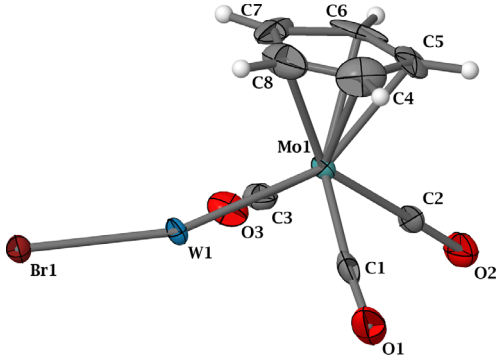

Figure 31
The high-resolution static figure displays the principal ellipses more clearly.

to select a particular orientation before implementing the full rendering.

Note that the default loading renders hydrogen atoms as small spheres, but the **ellipsoid** tab provides options for suppressing the display of H atoms altogether, or of showing their ellipsoids.

Note also that the ellipsoid properties are assigned to all the atoms in the current selection. This means that you could select different parts of the structure and supply them with different probability ellipsoids, or as simple spheres or sticks (useful, for example, in de-emphasising large ellipsoids associated with poorly refined solvent molecules). Such selective modifications should of course be detailed in a caption.

Another useful option is the ability to colour 'by temperature'. In practice, this is a graduated colour scale running from blue ('cold') through red to white in accordance with the modulus of the displacement amplitude. It can provide additional visual cues to interpreting the displacement behaviour of the atoms in the structure.

Fig. 32 shows a view of the structure normal to the cyclopentadienyl ring. Here the ellipsoids are shown at 60% probability, coloured in proportion to their mobility. The ellipsoids have also been made translucent, so that one may see embedded atom spheres, colour coded by element. The torsional motion of the Cp ring is clear, and especially its asymmetric nature. The relatively large motions of the two terminal oxygens are also immediately obvious.

7.3. Complementary styles of representation

This example shows how to produce an unusual representation illustrating the molecular displacements of the crystal packing (Fig. 33). We simply outline the procedures here; reproducing the details is left as an exercise for the reader.

On the **crystallography** tab, select a cell packing range ($2\times2\times1$ was chosen in this example). The default cell packing rendering is ball-and-stick; leave that unchanged. Using the **select/label** tab, select the individual molecules surrounding the one that you wish to emphasise. Assign them 100% van der Waals atom radii and colour them distinctively. It may be necessary to select one of the space-filling molecules and conceal it in order to see the molecule of interest sitting in the pocket formed by its neighbours. There are several ways of hiding a molecule, some of which interfere with other items in a current selection. Perhaps the safest way is to select the molecule, then choose 'atoms off' and 'bonds off' for that molecule.

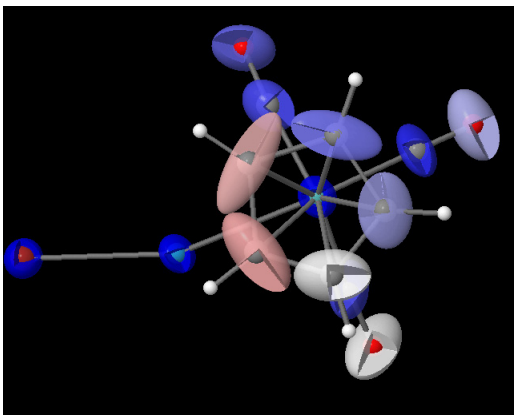

Figure 32
Use of colour and higher-probability ellipsoid envelopes to emphasise the mobility within the compound.

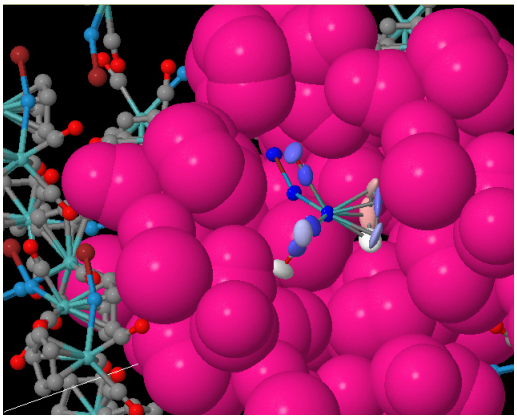

Figure 33
Molecular motions within the cell packing.

Finally, deselect everything and then select the central molecule. Using the **ellipsoid** tab, render 60% probability ellipsoids and colour the molecule by displacement modulus.

When you are happy with the result, save the current view into a button script (see Fig. 13) and enter a suitable caption. Now save the new view using the secondary save button ('Save updates to scripts only').

The result not only illustrates how an individual molecule is free to rotate and stretch within the steric constraints of its neighbours, but allows the reader to zoom out and appreciate how the molecules sit in relation to the large-scale order of the crystal symmetry.

8. Tutorial 4: a biological macromolecule example

This tutorial uses the structure of the SH3 domain of rat endophilin A2 (Loll *et al.*, 2008). Start the application with the PDB code 3c0c. By default the toolkit provides a cartoon representation of the structure (Fig. 34).

8.1. Arrangement and labelling of an initial view

To accentuate the colour range of the cartoon, go to the **select/label** tab, select 'backbone' under the list of protein-specific options. Then go to the **structure** tab and toggle the 'cartoon' checkbox off and on to extend the colour gradient across the whole backbone from blue at the N terminus to red at the C terminus. You may also like to try out the other schematic structural representations available on this tab. Note that they are additive, and can be assigned separate colour schemes and translucencies. This allows you to superimpose different interpretations of the structure on the one view.

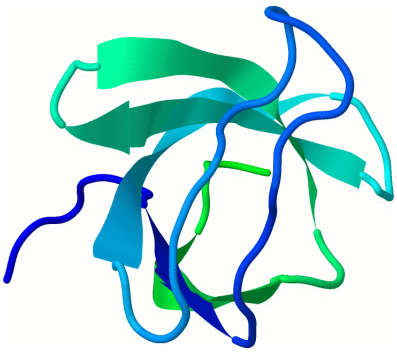

Figure 34
Default cartoon representation upon loading a protein structure.

For now, return to the cartoon view, manipulate the molecule into a preferred orientation, and zoom in to fill the visualization window as much as possible (Fig. 35). Save this using the 'Primary save' button (Fig. 5) as the initial view of the enhanced figure.

Next add some labels to the figure. The **select/label** tab is helpful in allowing you to select certain components of the structure, and in a limited amount of labelling (mostly by atom name or by element). For more complex labelling, you will need to work in the *Jmol* console window; or in the **scratch** tab, where you can build up and test a complex labelling script. We illustrate that approach here. You may also find it helpful to review Section 6.5, where more details are given about how you can carry out the 'detective work' of retrieving the effects of clicking on toolkit buttons and menus from the *Jmol* console history function, and then modify them to your specific needs. Of course, to achieve everything you want to do, you will need to combine this approach with reading the *Jmol* documentation.

Begin by labelling the molecular termini with their sequence numbers. If you allow your cursor to hover over an atom, then, after a slight delay, a popup appears that identifies the atom, including information about its residue type and sequence number. If you do this, you will find that the blue (N) terminus is

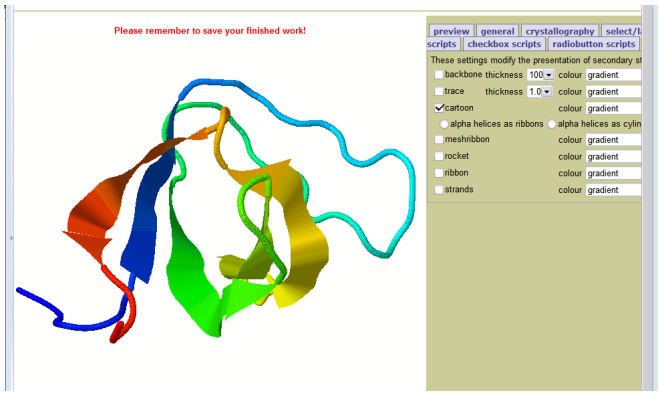

Figure 35
Protein structure after colour enhancement, reorientation and scaling.

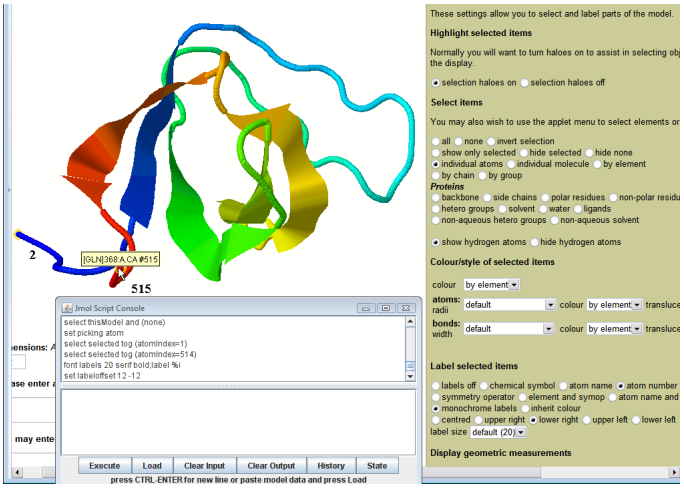

Figure 36
Using mouse hover, console history and selected radiobutton actions to deduce an appropriate script.

residue number 305, the red (C) terminus number 368. You will also see the sequential numbers of the terminal atoms (respectively numbers 2 and 515), which can be used as identifiers for anchoring the desired labels.

Fig. 36 shows this mechanism in operation. It also shows how you can use the **select/label** tab to select the terminal atoms and label them with their sequential numbers, and then recover from the *Jmol* console the scripting commands that have been put into effect in doing so.

The script retrieved by following these steps is shown in the history window of the console in Fig. 36, and is:

```
select thisModel and (none)
set picking atom
select selected tog (atomIndex=1)
select selected tog (atomIndex=514)
font labels 20 serif bold;label set labeloffset 12
-12
```

Note a few things here. *Jmol*'s internal script commands use the atomIndex identifier, which is offset by 1 from the atomNo that shows up in the hover labels. The select commands are executed in the context of your interaction through the toolkit. To provide the reader with a more robust script, it would be good practice to wrap your script in a save/restore pair of commands that separates the selections needed in the labelling process from whatever other selections are in effect. The 'set picking' command will not be needed in a non-interactive script: it was invoked only to allow you to pick interactively the atoms that you wanted to label. Finally, the 'label %n' command selects the atom sequential number. It can be replaced by 'label %r' to print the residue number (or, if you do are not familiar with that notation, you could specify individual literal strings as labels).

Putting all these ideas into effect, and extending them to other aspects of the figure that you want to label, you could end up, after a little trial and error, with a script such as the following:

```
save selection ORIG;
color labels black;
select (atomNo=2);
```

```
font labels 20 serif bold;label %r;
set labeloffset 0 -12
select (atomNo=515);
font labels 20 serif bold;label %r;
set labeloffset 12 -12

select (atomNo=95);
font labels 32 sanserif italic;label "RT loop"
select (atomNo=286);
font labels 32 sanserif italic;label "Src|loop"
set labeloffset -20 0;

restore selection ORIG;
```

The 'save' and 'restore selection' commands isolate this labelling from other actions; 'color labels black' creates black labels (actually, labels that contrast with the background, so they will automatically become white against a black background). The vertical bar in the string label 'Src|loop' splits the label over multiple lines at that point.

Fig. 37 shows how this can be developed in the **scratch** panel.

When you are happy with the result, copy and paste this script into one of the script input boxes on the **checkbox scripts** tab. You should also provide a script that has the opposite effect (*i.e.* to remove the labelling) and a caption, *e.g.* 'Label major features'. A suitable counter script for action when the checkbox is unchecked would be:

```
save selection ORIG;
select (atomNo=2); label off;
select (atomNo=515); label off;
select (atomNo=95); label off;
select (atomNo=286); label off;
restore selection ORIG;
```

Finish this lesson by adding another simple pair of checkbox scripts, 'stereo 5 on;zoom 75%;' and 'stereo off;zoom 120%;' to produce a wall-eyed stereo representation (the '5' is the number of degrees divergence between right and left eye view – you may make this a negative number for cross-eyed stereo viewing). The zoom factors are determined empirically to fill the available space. With both enhancements activated, you have reproduced the features of the published Fig. 1 of Loll *et al.* (2008).

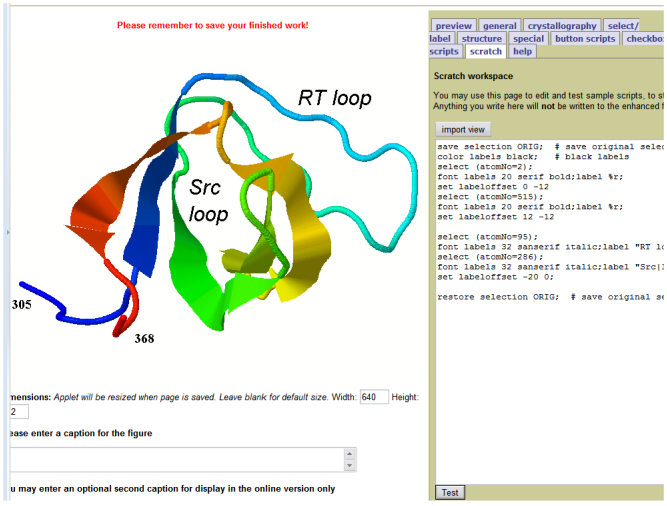

Figure 37
Developing a labelling script in the scratch window.

8.2. Lesson 2: highlighting surface features.

Fig. 2 of Loll *et al.* (2008) is a surface representation of the molecule, colour coded by element. *Jmol* allows you to draw a molecular surface *via* an option on the **general** tab, but although the surface can be drawn in many colours, it does not inherit the colouring by element of the underlying atom species. However, you can emulate the required effect by making the surface translucent, and placing a space-filling model below, colour-coded by element.

Fig. 38 is constructed from a recipe that involves selecting all atoms at 75% van der Waals radii, coloured by element and with 80% translucency (from the **select/label** tab), and a molecular surface coloured 'metal' at 60% translucency from the **general** tab. A black background has also been selected (from the **general** tab) The colours can be emphasised, if desired, by reducing the level of translucency. However, if one then selects the option 'Label major features' that you created in the last lesson, the labelling will be concealed almost completely. It is found by experimentation that these values provide a reasonable compromise to optimise the visibility of surface, coloration and labels.

The complete view is associated with a button using the 'import view' function on the **button scripts** tab, and a suitable caption composed.

The published article identifies the Trp 343 residue as a convenient geographical marker for the ligand-binding groove. You could therefore provide another checkbox script allowing the reader to switch on and off highlighting of that residue. A suitable activation script is:

```
save selection ORIG;
select none;
select (resNo=343);
atoms cpk 90%;
colour atoms magenta;
select none;
restore selection ORIG;
```

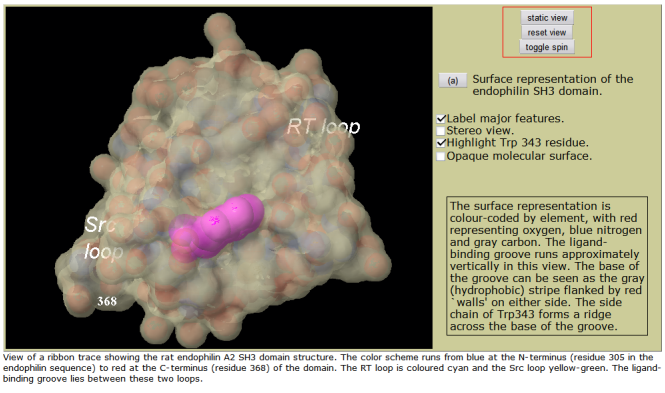

Figure 38
The surface representation overlaid with labelling and highlighting options.

You could also add another checkbox to toggle the molecular surface between translucency and opacity. The opaque view ('colour isosurface opaque;') loses the element colour-coding, but will render faster, which will be helpful if the reader wishes to rotate the structure, or has a relatively slow computer.

If the reader also activates the options to toggle spin on and to display a stereo view, a very convincing three-dimensional impression is obtained on a sufficiently fast computer.

9. Toolkit options reference

All the options presented in the toolkit interface are described for the beta 2 release version of the *Jmol* toolkit. Significant changes to these may follow user feedback during the beta test phase.

*9.1. The **preview** tab*

This is the first tab, and is the one that is open when you load (or reload) the editor page (Fig. 39). It allows you to preview the effect of the scripts associated with the enhanced figure. When a structure is first loaded, it contains two of the standard buttons that will always be created for an enhanced figure.

'Reset view' reloads the initial view that is saved whenever the 'Primary save' option is selected. This is also the view that is recorded as a static image for incorporation into the PDF edition of the journal. (The online enhanced figure also contains a 'static view' button that shows this static figure. It is absent from the **preview** pane since it serves no useful purpose here.)

'Toggle spin' rotates the view if it is stationary, or stops it if it is currently rotating. Since this is one of the most common requirements of an enhanced figure, it is provided as standard.

Below these buttons, any scripts that you create and link to buttons, checkboxes or radio buttons will appear, to allow you to test their effects before saving the enhanced figure.

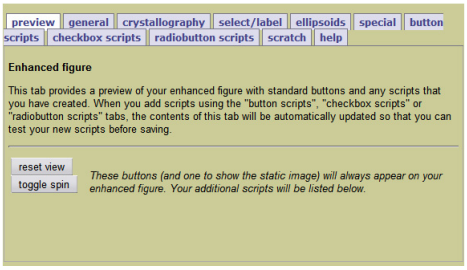

Figure 39
The **preview** tab

*9.2. The **general** tab*

This tab provides options to change global aspects of the figure (Fig. 40). In general you will start here.

`black background`

A check box to select a black background in the visualization window. Other background colours may be set from within the applet using the *Jmol* menu. By default, a white background is set, in the style of traditional static figures. Black may be selected to emphasise colour or translucency effects. Other background colours will not usually be accepted unless there is a compelling reason.

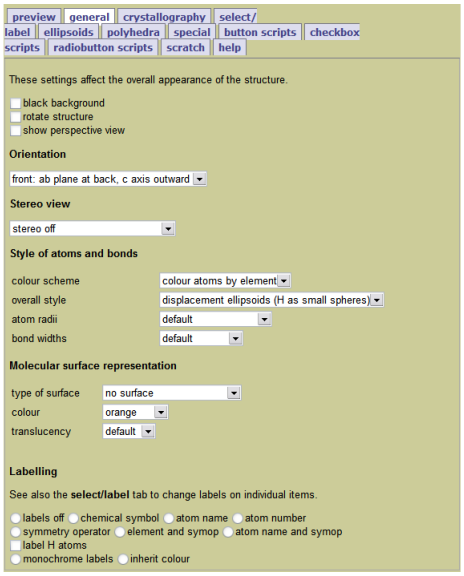

Figure 40
The **general** tab

`rotate structure`

A checkbox allowing rotation about a vertical axis in the plane of the image (around the *y* axis). This is a useful feature to allow the author to see how a rotating structure will appear. Normally, however, you will unset this option before saving, so that the preferred orientation is saved in the static image. Note that the enhanced image page will *always* have a 'toggle spin' button, so that the reader may always choose a rotating view.

`show perspective view`

A checkbox to force a linear perspective depth representation. The *Jmol* default setting 'set cameraDepth 3.0' may be modified using the console if a more or less exaggerated perspective is required.

9.2.1. Orientation A menu specifying projections along the main crystallographic axes. *Jmol* uses the designations 'front', 'back', 'left', 'right', 'top' and 'bottom', which are explicitly described in the menu options.

9.2.2. Stereo view A menu allowing stereoscopic views to be set up as side-by-side (cross-eyed or wall-eyed) pairs, or as red/blue, red/cyan or red/green superimpositions.

9.2.3. Style of atoms and bonds

`colour scheme`

The menu options are 'by element' (the default for small molecules and inorganics), 'by alternative location' (typically

where positional disorder is present), 'by the molecule', 'by formal charge', and 'by thermal displacement'. Biological macromolecules also have 'by amino acid', 'by secondary structure' and 'by chain'. The default for biological macromolecules is to colour residues along a rainbow gradient, from blue (at the N or 5′ terminus) to red (at the C or 3′ terminus). Other colouring schemes for macromolecules are available in the **structure** tab.

`overall style`

The common menu options are 'ball-and-stick', 'stick, 'wireframe' and 'CPK Spacefill'. For inorganic and small-molecule structures there are also 'displacement ellipsoids' and 'displacement ellipsoids (H atoms as small spheres)'. For proteins there are also 'cartoon' (the default), 'ribbon' and 'strands'. Additional abstract representations are available for biological macromolecules through the **structure** tab. Note that if you wish to display a crystallographic packing diagram, you should first set up the desired view using the **crystallography** tab, then return here to change the rendering style.

`atom radii`

This menu allows a number of settings of atomic radii, either as a fraction of the van der Waals radius, or proportional to the ionic radii. 'default' for small-molecules and inorganics is 20% of the van der Waals radius. For macromolecules, atom and bond rendering is off by default (since the usual starting representation is a cartoon or other abstract view).

`bond widths`

The menu provides a number of bond width values in ångström units. The default for inorganics and small molecules is 0.15 Å. For macromolecules, the default is to turn bonds off – this means that they must explicitly be turned on in this menu if a 'vine' or 'ball-and-stick' representation is desired.

`hydrogen bonds`

(*Biological macromolecules only.*) The menu allows you to select whether hydrogen bonds are displayed or not, and a bond width to assign to them. In the current release of *Jmol*, 'hydrogen bonds' are currently limited to certain types of calculated bonds in biological macromolecules, specifically: (*a*) between protein amide NH and protein amide carbonyl oxygens and (*b*) between nucleic acid base pairs.

`disulfide bonds`

(*Biological macromolecules only.*) Specifies whether disulfide linkages are shown, and what radii (in Å) they should have.

9.2.4. Molecular surface representation These options allow the display of a number of slightly different molecular envelopes.

`type of surface`

The 'van der Waals' surface is formed from the individual atomic van der Waals radii. The 'solvent' surface is that traversed by a spherical probe that rolls over the currently selected atoms. The 'solvent-*accessible*' surface is the locus of the centre of a spherical probe that rolls over the currently selected atoms. For these two cases the radius of the probe is taken to be the default *Jmol* radius of 1.2 Å; it may be changed in the *Jmol* console using the 'set radius' command. The 'molecular' surface is the same as the solvent surface for a probe of fixed radius 1.4 Å. The 'dot surface' option renders the surface by discrete dots.

`colour`

Sets the molecular surface to a selected colour. If the surface is represented by dots, these will retain colouring by element. This behaviour may be changed, if necessary, by issuing a 'colour dots' command within the console.

`translucency`

A menu allowing levels of translucency to be set from 0 (opaque) to 100% (invisible) for the molecular surface.

9.2.5. Labelling A number of options are presented to modify the labelling conventions for the figure as a whole. These would normally only be of use for a single, relatively small, molecule. To label individual atoms or parts of the structure, one should use instead the options on the **select/label** tab. The options available fall into three groups.

`labels off`
`chemical symbol`
`atom name`
`atom number`
`symmetry operator`
`element and symop`
`atom name and symop`

The options are largely self-descriptive. 'Atom number' is a sequential number assigned by *Jmol*; 'atom name' is the label found in the CIF. Symmetry operators are given in the form 2556, for example, where the '556' represents the cell offset from the base coordinate set at 555 (*i.e.* in this example it refers to a translation of one unit cell along the **c** axis). The initial integer is the sequence number of the symmetry operation in the ordered list in which it appears in the CIF – *i.e.* here, symmetry operation number 2. In line with current journal policy, these labels are applied only to non-hydrogen atoms.

`label H atoms`

Provides an option to label H atoms. In this case, all atoms are labelled by atom name. To change this behaviour, one should select individual atoms and label them using the options available on the **select/label** tab.

`monochrome labels`
`inherit colour`

By default, *Jmol* creates labels in the same colours as their parent atoms. The 'monochrome' option allows a global choice of black on a white background (the usual journal default for printing) or white on a black background.

*9.3. The **crystallography** tab*

This tab provides options for generating crystal packing diagrams and for identifying or annotating symmetry-related features (Fig. 41). It is a good starting place if the main objective of your figure is to show the crystal packing.

`unit cell`
`show cell parameters`
`hide cell parameters`

An outline of the unit cell may be drawn or hidden. By default, it is generated when small-molecule and inorganic compounds are first loaded, but not for biological macromolecules.

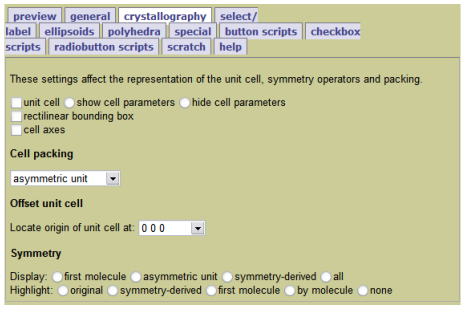

Figure 41
The **crystallography** tab

A legend displaying the space group and cell parameters may be displayed in the top left-hand corner. By default, IUCr journal style is *not* to display this information.

9.3.1. Cell packing The menu provides a list of options to display: the asymmetric unit only; the unit-cell contents when all symmetry operations have been applied (this will display atoms lying outside the basic unit-cell boundary); the contents of the central cell of an extended lattice (this will show only atoms located within the unit-cell boundaries, which may of course include portions of symmetry-generated molecules that lie mostly in adjacent unit cells); and a selection of planar or cubic packing nets. The limit provided in the menu is $3 \times 3 \times 3$ unit cells. More extended lattices can be generated using the console, but you should remember that the computational demands in generating and manipulating large numbers of atoms in real time may make this impractical for readers with limited computing facilities.

9.3.2. Offset unit cell The menu allows the unit cell to be relocated.

9.3.3. Symmetry A small number of utilities are provided that allow you to display or highlight part of the symmetry-generated contents of the crystal lattice.

```
Display:  first molecule
asymmetric unit
symmetry-derived
all
```

Various portions of the lattice are displayed. 'First molecule' examines the list of atoms, applies bonding rules to identify one or more discrete molecules, identifies the molecule that is first in the list (*i.e.* that contains the atom numbered 1 in sequence), and shows all symmetry mates of that molecule. The *Jmol* command that is executed to achieve this effect is 'restrict within(molecule,atomno=1)'. Another molecule may be chosen by specifying a suitable atom sequence number in the console.

'Asymmetric unit' displays only the atoms occupying the asymmetric unit; no symmetry operations are applied. 'Symmetry-derived' displays the symmetry mates to the asymmetric unit; 'all' displays the complete contents of the lattice.

```
Highlight:  original
symmetry-derived
first-molecule
by molecule
none
```

These options are largely complementary to the previous set. Instead of displaying or hiding parts of the lattice, they highlight the selected items with different colours.

*9.4. The **select/label** tab*

This is possibly the most useful tab in allowing you to highlight particular portions of the structure. It is also at first glance the most complicated. However, the various options are collected into logical groups, and you will only need to use the ones that are relevant for your purpose (Fig. 42).

You can also, of course, simply use the selection options available through the *Jmol* pop-up menu, or perform explicit selection, labelling and measurement commands through the *Jmol* console.

Note that the options on this page invoke either or both of the *Jmol* 'select' and 'set picking' sets of commands, often in complex ways. When you have finished working with these options, we recommend that you click the buttons 'all' (under 'Select items') and 'enable measurements' (under 'Display geometric measurements'). You cannot select both together, but if you click on each in turn, you will restore the behaviour of *Jmol* to the one with which most users will be familiar (*i.e.* all atoms are selected, and the user may click on atoms to measure distances and angles between them).

9.4.1. Highlight selected items

```
selection haloes on
selection haloes off
```

It will be much easier to understand what atoms will be affected by a command if you turn selection haloes on – each atom selected will be surrounded by a yellow sphere. Normally you will want to turn selection haloes off when you have finished manipulating the molecule, so that they do not appear in the static figure.

9.4.2. Select items The options in this section allow you to select particular parts of the structure, and to show or hide the parts selected.

```
all
none
```

These are global settings. When you have finished working on this page, you should normally select 'all' so that any operations that the reader performs through the standard *Jmol* menu will have the anticipated effect of acting on the structure as a whole. By default, all the atoms will initially be selected, so you may wish to select the 'none' option *before* you begin to select individual atoms or groups of atoms.

```
invert selection
show only selected
hide selected
hide none
```

Figure 42
The **select/label** tab

These options affect the display of the selected objects, and allow you to invert the sense of selection – *i.e.* to select the complementary set of objects.

```
individual atoms
individual molecule
by element
```

These options establish the 'picking mode' that allows you to make interactive selections by clicking on objects in the structure with your mouse. If you click on 'individual atoms' then each mouse click will add another atom to the set selected (clicking a second time on any atom removes it from the selection set). The 'individual molecule' setting will select all atoms in the same molecule as the one that you click on (note that the 'molecule' will be that established by *Jmol*'s own connection rules). The option 'by element' selects all atoms of the same elemental type as that clicked on. These actions are additive – if you select 'by element' and click on a C atom, then an N, all carbon and nitrogens will be selected. They are also reversible – if you decide that you didn't want the carbons, click again on a C atom and all will be deselected.

(*Biological macromolecules only*)

```
backbone
side chains
polar residues
non-polar residues
hetero groups
solvent
water
ligands
non-aqueous hetero groups
non-aqueous solvent
```

Several options are provided to help in selecting portions of a protein or nucleic acid structure, including solvent water molecules, all solvent (including free phosphate and sulfate ions), hetero groups and ligands, and particular components of the polypeptide or polynucleotide molecules. Note that they all rely on correct designation of these components in the loaded mmCIF.

```
show hydrogen atoms
hide hydrogen atoms
```

Because it is very common to suppress H atoms from display, a separate option is provided to display or hide all hydrogens.

9.4.3. Colour/style of selected items Once you have made a selection, you will usually wish to change some aspects of its representation.

```
colour
```

This option provides a selection of colours, as well as 'translucent' (70% translucency) and 'opaque'. The colour applies to all items selected, which may not always be what you want. If you select two atoms and a connecting bond, and change the colour of the selection by this menu, the selected atoms and the bond between them will change to the desired colour. However, by default *Jmol* colours a bond in two halves, each corresponding to the colour associated with the atom immediately adjacent. If you use this option to change the colour of a selected C atom from grey to red, for example, you may be surprised when the other bonds from the selected carbon also change to red. In that case, you will wish to use the other options in this section for more control over individual atoms and bonds.

```
atoms:  radii
colour
translucency
```

These options provide greater control over the atomic spheres in the selection. You may change their radii, colours and translucencies through a range of values.

```
bonds:  width
colour
translucency
bond order
```

These options provide greater control over the bonds in the selection. You may change their widths, colours and translucencies through a range of values. You may also assign different representations corresponding to an assigned bond order – single, double, aromatic *etc*. You may hide individual bonds. Note that you may also use these options to draw a line between any two atoms – no checking is done as to whether the connection satisfies chemical bond length constraints. To do this, first 'select none', then 'select by individual atoms'; click on the two atoms you wish to connect, and then select under the 'bonds: width' menu the option 'connect all selected'.

9.4.4. Label selected items These options allow you to label individual atoms or groups of atoms, and to make limited changes to the style of the label. Note that the labelling styles offered by *Jmol* do not always correspond to the requirements of the IUCr journals, so labelling should be used sparingly, particularly on the main figure (which will be published also in the PDF edition of the journals).

```
labels off
```

chemical symbol
atom name
atom number
symmetry operator
element and symop
atom name and symop

These specify the content of the label, and are largely self-explanatory. 'Atom number' represents the sequence number of the atom in the coordinate list, and is probably of little use in a publication. See also §9.2.5 for discussion of the format of the labels.

monochrome labels
inherit colour

By default, *Jmol* renders atom labels in the same colour as their parent atom. IUCr journals prefer black labels (on a white background) or *vice versa*, which are supplied by the 'monochrome labels' option.

centred
upper right
lower right
upper left
lower left
label size

A number of standard offsets are provided for the label. If these are not sufficient to prevent the label colliding with some other object, you may wish to use a scripting command such as 'set labeloffset 12 0' to set the label 12 pixels to the right of the atom (the arguments to the 'set labeloffset' command are the *x* and *y* displacements in pixels; 12 is the default value).

The label size may also be changed; 20 pixels is the default value.

9.4.5. Display geometric measurements One of the most useful features of *Jmol* as a visualization tool is the ability for the user to click on two, three or four atoms and see a representation of bond distances and angles. This is achieved by the default setting 'select picking measure', which will be turned off if you have used any of the options provided for selecting individual atoms or groups through mouse clicks. If you have done so, you should click on the 'enable measurements' option on this tab before saving what you have done (unless you intend the reader to use the select picking mode currently in use).

These options also allow you to render some geometric information in your saved enhanced figure.

enable measurements
delete measurements
colour
linewidth
font size

To draw measurements between two atoms, select the 'enable measurements' option and click once on each of the atoms. To select three or four atoms, double-click on the intervening ones.

You may set the colour and line width (in Å) of the measurement lines, and the font size (in pixels) of the associated labels. If you select 'hide' on the font size menu, you may use this technique as an alternative way to draw lines between arbitrary atoms. Note that the 'thin dotted' menu item under the 'linewidth' option allows you to draw a dotted line; *Jmol*, however, does not currently provide options for changing the width of such a dotted line.

9.4.6. Special features

centre selected atom
rotate about selected atom
stop rotation

These options are occasionally useful for recentring the view on a specific atom. 'Rotate about selected atom' locates the rotation axis on the selection, and causes the structure to rotate about that axis, so that you can check that it behaves as expected. You may wish, however, to 'stop rotation' in order to save a specific initial view. The reader will always be able to restart the rotation using the standard 'toggle spin' button on the enhanced figure.

*9.5. The **ellipsoids** tab*

(*Inorganic and small-molecule compounds only.*)

These options allow you to change the style of atomic displacement ellipsoids (Fig. 43).

probability(%)

The probability envelope represented by the ellipsoids.

style

Jmol offers a wide choice of representations. The default (cutout octants with axes) displays *ORTEP*-style ellipsoids; the principal ellipses can be distracting especially against black backgrounds, and may be inhibited using the simple 'cutout octants' style. Other options allow increasingly schematic views of the ellipsoids, or in the case of 'intersecting axes' the axes only. Some of the representations can be combined.

colour
translucency

A selection of colour and translucency schemes may be applied. Colour 'by temperature' applies a graduated scale from blue through red to white for atoms with progressively greater displacement modulus.

hydrogen atoms

H atoms may be represented as small spheres (the default); with ellipsoids if the refinement warrants it; purely by position (*i.e.* shown as capped sticks); or suppressed altogether.

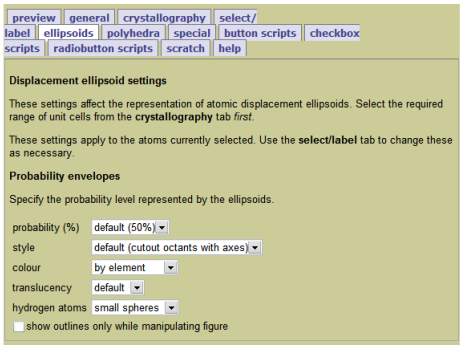

Figure 43
The **ellipsoids** tab

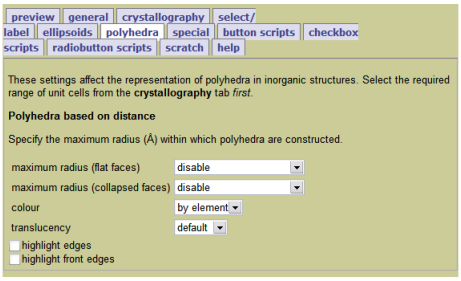

Figure 44
The **polyhedra** tab

show outlines only while manipulating figure

Because of the high computational effort needed to render ellipsoids, it can take time to move the molecule around. If you select this option, the ellipsoids will be shown in outline only during manipulations of the figure, making it much easier to decide an optimal view direction.

*9.6. The **polyhedra** tab*

(*Inorganic compounds only.*)

These options allow limited control over the display of coordination polyhedra in inorganic structures (Fig. 44). For more control, you should consult the detailed *Jmol* documentation.

9.6.1. Polyhedra based on distance The current menus support coordination polyhedra with a variable number of vertices based on the radius from a central atom.

maximum radius (flat faces)
maximum radius (collapsed faces)

Normally you will wish *Jmol* to calculate polyhedra based on default bond lengths. The optional radii, which extend from 1.0 to 5.0 Å, may nevertheless be useful for constructing polyhedra of a desired size around a selected subset of atoms in the crystal (use the **select/label** or **crystallography** tabs to make selections). The 'flat face' rendering draws convex polyhedra. 'Collapsed faces' draws concave figures, making it easier to see the central atom.

colour
translucency

These menus allow you to modify the appearance of the edges and faces of the polyhedra.

highlight edges
highlight front edges

These options emphasise the edges (or the visible edges) of the polyhedra to make their three-dimensional outlines clearer.

*9.7. The **structure** tab*

(*Biological macromolecules only.*)

These options determine the style of various schematic representations of secondary structure in proteins and nucleic acid molecules (Fig. 45). They can be applied to portions of the structure previously defined by options on the **select/label** tab.

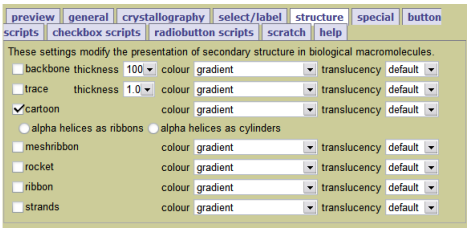

Figure 45
The **structure** tab

backbone
trace
cartoon
  alpha helices as ribbons
  alpha helices as cylinders
meshribbon
rocket
ribbon
strands

The 'backbone' representation draws a zigzag line through the α carbon atoms of polypeptides or the P atoms of polynucleotides. The thickness may be set from the menu using a range of values expressed in *Jmol*'s internal dimension units (250 units = 1 Å). The 'trace' is a smooth curve interpolated between the α carbon or phosphorus atoms. In this case the thickness may be selected from a range of values in Å units.

The 'cartoon' representation uses ribbons with an arrowhead for α helix and β strand stretches, and trace for the remaining turns, loops and random coils. For nucleic acids, the nucleotides are displayed as flat molecular templates. The rendering may be modified to show 'alpha helices as cylinders', *i.e.* as arrowed cylinders in the style of 'rockets'. The 'rocket' representation displays only polypeptides; it uses arrowed cylinders for α helices, straight 'planks' with an arrowhead for β strands, and trace for the remainder.

'Ribbon', 'strands' and 'meshribbons' display ribbons following the trajectory of the interpolated curve that defines the trace. They employ respectively solid ribbons, ribbons made of parallel threads, or ribbons made of crossing threads. All may be used for polypeptides and polynucleotides.

The available colour schemes for each of these representations are: 'by element' (so that proteins appear grey from the α carbons, nucleic acids orange from P); 'by amino acid' (bright colours are used for polar amino acids, dark for hydrophobic ones; nucleosides all have the same brown colour); 'shapely' (an alternative colouring scheme used by *RasMol* and other software to colour residues by amino acid property; nucleosides are also coloured); 'by secondary structure' (helices are pink, β strands or sheets yellow, turns in blue, the remainder white; DNA and RNA are coloured purple and red); 'by chain'; and 'gradient' (a rainbow from blue at the N or $5'$ terminus to red at the C or $3'$ terminus). Each selection may also be coloured from a menu of single hues.

In addition, each representation can be assigned a translucency.

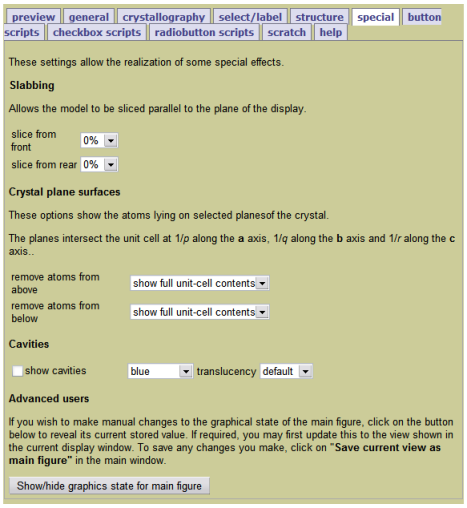

Figure 46
The **special** tab

*9.8. The **special** tab*

The **special** tab (Fig. 46) provides a small collection of 'special effects' achievable through *Jmol* scripting. The intention is not necessarily to provide features that will be of widespread use, but rather to illustrate some of the more unusual functions that can be used to good effect to illustrate particular features of a structure. This selection may grow if users can suggest novel examples.

9.8.1. Slabbing The effect of this option is to slice the model through a plane parallel to the plane of the display. It has the effect of a 'bacon slicer', removing the top or rearmost portion of the model, and is perhaps most effective when the model is rotating (and especially if rendered in some space-filling view).

```
slice from front
slice from rear
```

A range of values is provided for illustrative purposes. As with all the options on this tab, the author may use these as examples, and specify more precise commands through the use of the *Jmol* console.

9.8.2. Crystal plane surfaces This is similar to the slabbing mode, but it provides slices through a crystal structure parallel to particular Miller planes.

```
remove atoms from above
remove atoms from below
```

Again, the Miller planes available through the drop-down menus are for illustrative purposes only. Authors may wish to modify the indices to demonstrate a particular plane of interest in their structure.

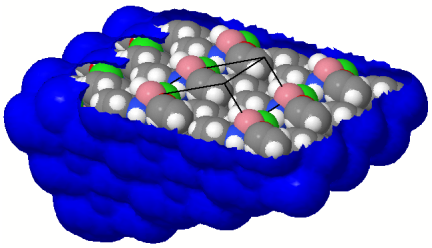

Figure 47
A slice through the crystal packing along the (202) plane displayed and highlighted using options from the **special** tab.

9.8.3. Cavities

```
show cavities
colour
translucency
```

In this version of the toolkit, the 'show cavities' option is essentially equivalent to the solvent-accessible surface that can be drawn on the **general** tab. It is hoped in future releases to include the cavity slabbing facility beautifully demonstrated on Alan Hewat's web page at http://icsd.ill.fr/slabslider/slab3d.html.

Fig. 47 shows an example of what is achievable using some of the options on the **special** tab.

9.8.4. Advanced users The final option on the **special** tab (Fig. 48) allows access to the stored graphics state of the main figure. It is the information that was stored when the last save was made using the primary save button. Its main use would be to restore the saved view without reloading the application, using the 'Activate' button at the bottom of the text field (for example, if you wished to use the same starting view as the basis for a number of different views stored in the various button and checkbox scripts). It is also possible to replace the stored view with the current one using the 'Update state script' button. This is equivalent to making a primary save.

It is expected that this will be of use only to those who understand in some detail how the graphics state may be manipulated, and it is therefore concealed from view unless the user specifically wishes to display it.

*9.9. The **button scripts** tab*

This tab (Fig. 49) provides space for the author to supply up to four *Jmol* scripts that will be associated with buttons on the enhanced figure page. The buttons will be labelled (a), (b), (c) and (d). Each script has an associated caption, which you should also supply through this tab.

Against each script field (on this and the other script tabs) is a button, 'import view', which will transfer the graphics state of the current view in the visualization window into the script box. This means that you can use all the options on the other tabs to generate a completely new view of the structure, which you can store as one of the scripts that you supply for the reader to run. Be aware, however, that this can create a very large script; and also that it will *completely* define the graphics state of the

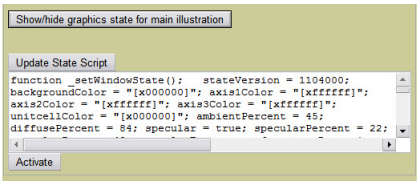

Figure 48
Access to the saved graphics state through the 'Advanced users' option of the **special** tab

visualization, which might conflict with some of the settings that you attempt to provide through other scripts.

The software places no constraints on what *Jmol* scripts you may load in these fields. They can be very simple indeed ('stereo on'); they can be complex views created using the tools in this toolkit and imported through the 'import view' button; or they can be arbitrarily complex scripts involving animations and other advanced features of *Jmol* provided by an expert.

However, it is important to meet the reader's expectations of what will happen when the various mechanisms for activating these scripts are used. The scripts on the current tab are associated with buttons on the enhanced figure page. The reader will not be surprised, when a button is clicked, if a completely new view of the structure is presented, or some 'one-off' animation is run. Therefore, these button scripts should be used when you wish to demonstrate quite distinct views of the structure. They may be the ones that rely most on the 'import view' facility to allow you to set up quite complex views that are very different from that of the main figure.

If, on the other hand, you want the reader simply to be able to change aspects of the structure that they are currently viewing, it may be better to create smaller scripts that are accessed as checkboxes or radio buttons (see the descriptions of the other script tabs for further discussion of this point).

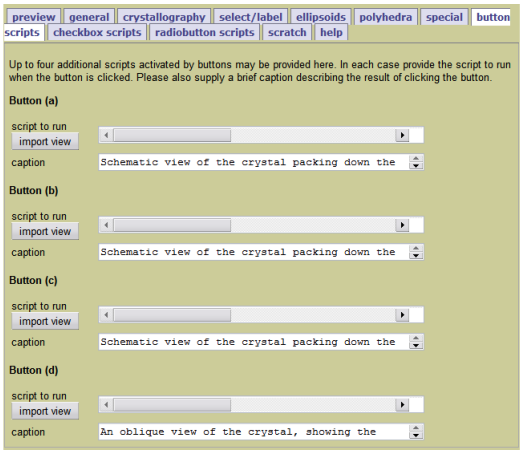

Figure 49
The **button scripts** tab

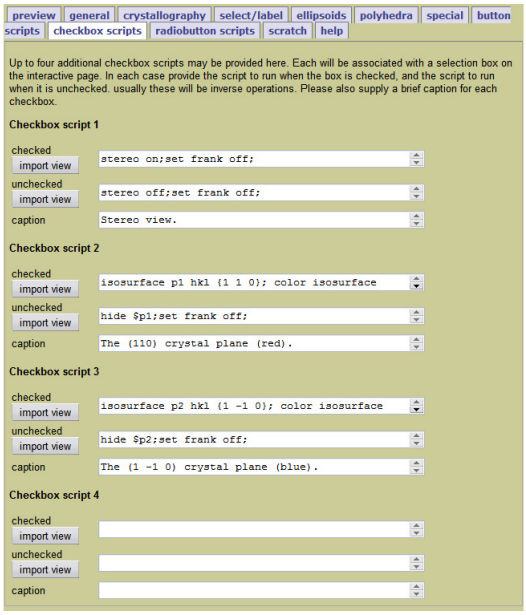

Figure 50
The **checkbox scripts** tab

*9.10. The **checkbox scripts** tab*

This tab (Fig. 50) provides space for the author to supply up to four *Jmol* scripts that will be associated with checkboxes on the enhanced figure page. Normally, you will supply a script to run when the checkbox is selected, and another to run when the checkbox is *un*selected. In keeping with the principle that the reader's expectations should not be upset, you will probably want to provide complementary on/off functions through these paired scripts ('stereo on', 'stereo off' *etc.*).

Supply a caption for each checkbox that you create.

You will normally to use checkboxes to provide the reader with features that can be turned on or off independently of other aspects of the current view, and that therefore are 'additive'.

As with other script fields, you may import the current view from the visualization window using the 'import view' button alongside each script field. In general, though, you will probably want to provide more lightweight *Jmol* scripts using this tab. See §6.4 for some suggestions on how to go about this.

*9.11. The **radiobutton scripts** tab*

This tab (Fig. 51) provides space for the author to supply one or two groups, each with up to six *Jmol* scripts that will be associated with radiobuttons on the enhanced figure page. 'Radio buttons' are normally used in web forms to select one among a set of mutually exclusive options. You should therefore structure any scripts offered to the reader through this interface along the same principles.

Note that you are not *obliged* to do so; any *Jmol* script can be inserted in any of the script fields. However, the reader is likely to become very confused if your scripts do not behave in the exclusive manner suggested by the radiobutton interface.

In that spirit, you should arrange that the scripts you provide in each group of radiobuttons select mutually exclusive options

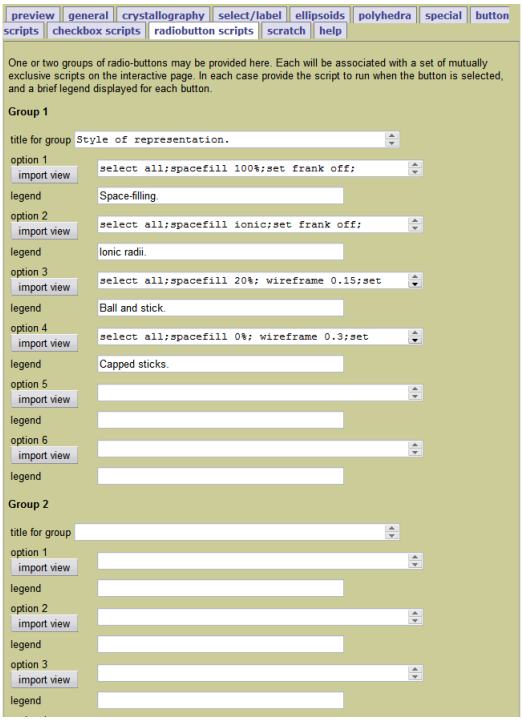

Figure 51
The **radiobutton scripts** tab

for a single feature. In the (optional) title for each radiobutton group, you can specify what that feature is.

As with other script fields, you may import the current view from the visualization window using the 'import view' button alongside each script field. In general, though, you will probably want to provide more lightweight *Jmol* scripts using this tab. See §6.4 for some suggestions on how to go about this.

*9.12. The **scratch** tab*

The scratch workspace (Fig. 52) is a text-entry field in which you can experiment with *Jmol* scripting. If you enter any commands in this box and then click the 'Test' button at the bottom, those commands are applied to the current view. The 'import view' button at the top of the scratch area imports the complete graphics state represented by the current view (note that this will completely overwrite anything already in the text entry box). This workspace can also be used as a convenient area into which to paste existing scripts, to test or modify them further.

The contents of the workspace are saved whenever either of the primary or secondary save buttons are clicked. This may therefore be used as a persistent notebook for storing ideas or experiments between editing sessions.

*9.13. The **help** tab*

The **help** tab provides a concise summary of how to use the software (Fig. 53).

10. Some *Jmol* resources

The *Jmol* home page at http://www.jmol.org has links to documentation, examples and further information. The *Jmol* scripting language is fully documented with interactive examples at http://chemapps.stolaf.edu/jmol/docs/. The book *How to use Jmol to study and present molecular structures Volume 1: Learning to use Jmol (basic and intermediate levels)* by Angel Herráez (ISBN 978-1-84799-259-8), available from www.lulu.com, is an excellent introductory primer.

Jmol has often been used in online tutorials. Many of these are indexed from the *Jmol* home page and can provide useful

Figure 52
The **scratch** tab

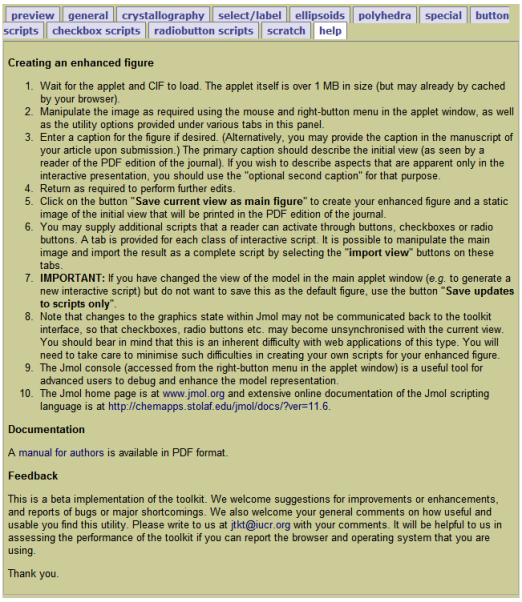

Figure 53
The **help** tab

hints on best practice in organising the information channelled through a *Jmol*-enhanced figure. The *Jmol* Tutorial-Authoring Template (JTAT) (http://bioinformatics.org/jmol-tutorials) is another valuable tool for developing authoring skills.

Professional *Jmol* scripting services are offered by Frieda Reichsmann of Molecules in Motion (http://www.moleculesinmotion.com/).

11. Acknowledgements

An early prototype of the toolkit was developed as part of a work-experience project with Tim Murray, a high-school student. Steve Cook provided the idea of displaying slices through different crystal planes. Simon Westrip solved a difficult issue regarding save functions. David Hoare helped with many JavaScript problems. Significant improvements to the user interface are due to Frieda Reichsmann, Rolf Huehne, Bob Hanson and Alan Hewat. Other members of the *Jmol* community have helped, knowingly or unwittingly, through their enthusiastic involvement on the jmol-users mailing list or by providing model applications. Many valuable suggestions have been received from the IUCr journal editors. I am grateful to all these people for their help and input.

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Appendix A
Useful *Jmol* commands

A.1. Basic mouse controls

For a full menu of options: click the right mouse button (CTRL + click on a Mac).

To zoom in or out: SHIFT + click and hold the left mouse button (SHIFT + click on a Mac).

To rotate compounds in 3D: click and hold the left mouse button (click on a Mac).

To rotate compounds in the plane of the screen: SHIFT + click and hold the right mouse button.

To move compounds in the plane of the screen: CTRL + click and hold the right mouse button.

A.2. Synopsis of Jmol commands

The following list of commands, with a synopsis of the most useful options, is taken from the *Jmol* scripting documentation at http://chemapps.stolaf.edu/jmol/docs/

```
animation ON/OFF{default: ON}
animation direction -1/+1
animation fps [frames-per-second]
animation frame
animation mode LOOP [time-delay1] [time-delay2]
animation mode ONCE
animation mode PALINDROME [time-delay1] [time-delay2]

axes ON/OFF{default: ON}
axes (decimal)
axes DOTTED
axes (integer)
axes MOLECULAR
axes UNITCELL
axes WINDOW

backbone ON/OFF{default: ON}
backbone [backbone-radius]

background [RGB-color]
background HOVER [color-none-CPK]
background LABELS [color-none-CPK]

bondorder 0.5, 1, 1.5, 2, 2.5, 3, 4, -1, -1.5, -2.5
bondorder [connection-options]

boundbox [atom-expression]{default: all atoms}
    [line-width-or-type]{default: ON}
boundbox [atom-expression-or-coordinate] [xyz-coordinate]
    [line-width-or-type]{default: unchanged}
boundbox CORNERS [atom-expression-or-coordinate]
    [atom-expression-or-coordinate]
    [line-width-or-type]{default: unchanged}

calculate AROMATIC
calculate HBONDS
calculate STRUCTURE
calculate SURFACEDISTANCE WITHIN [atom-expression]
calculate SURFACEDISTANCE FROM [atom-expression]

cartoon ON/OFF{default: ON}
cartoon [cartoon-radius]

center [atom-expression]
center [xyz-coordinate]
center [drawn-object]
center

centerAt ABSOLUTE x y z {default: 0.0 0.0 0.0}
centerAt AVERAGE x y z {default: 0.0 0.0 0.0}
centerAt BOUNDBOX x y z {default: 0.0 0.0 0.0}

color _color_name_or_scheme
color (atom object)
color [atom-associated-object] _color_name_or_scheme
color (bond object)
color BONDS [color-none-CPK]
color SSBONDS [color-none-CPK]
color HBONDS [color-none-CPK]
color HBONDS TYPE
color (element)
color [element-name] [RGB-color]
color [model-object] [RGB-color]
color (named object)
color [drawn-object] [RGB-color]
color (scheme)
color "colorSchemeName" RANGE [min] [max]
color measures [RGB-color]
color selectionHalos [color-none-CPK]
```

```
configuration [configuration number]

connect

console

data "label"
data CLEAR

define [variable-name] [atom-expression]

delay [time-delay]
delay on

depth

dipole

display [atom-expression]

dots ON/OFF{default: ON}
dots VANDERWAALS
dots IONIC
dots nn%
dots (decimal)
dots +(decimal)

draw [objectID] [modifying parameters] [positions]
draw DELETE
draw LIST

echo (string)

ellipsoid or ellipsoids
ellipsoid ON/OFF{default: ON}
ellipsoid nn%
ellipsoid [object id] ON
ellipsoid [object id] OFF
ellipsoid [object id] AXES {ax ay az} {bx by bz} {cx cy cz}
ellipsoid [object id] CENTER {x y z}
ellipsoid [object id] CENTER { atom expression }
ellipsoid [object id] CENTER $object
ellipsoid [object id] COLOR [color parameters]
ellipsoid [object id] DELETE
ellipsoid [object id] SCALE (decimal)

exit

font [object-with-text] [font-size]
    [font-face]{default: SansSerif}
    [font-style]{default: Plain}

frame (integer >= 1)
frame (decimal) / (decimal) - (decimal)
frame 0 / 0.0
frame ALL / LAST / NEXT
frame PAUSE
frame PLAY (starting frame)
frame PLAYREV (starting frame)
frame PREVIOUS
frame RANGE (starting frame) (ending frame)
frame RESUME
frame REWIND

frank ON/OFF

geoSurface ON/OFF{default: ON}
geoSurface VANDERWAALS
geoSurface IONIC
geoSurface (integer)
geoSurface (decimal)
geoSurface +(decimal)

getProperty animationInfo
getProperty appletInfo
getProperty atomInfo (atom expression)
getProperty atomList (atom expression)
getProperty auxiliaryInfo
getProperty bondInfo (atom expression)
getProperty boundBoxInfo
getProperty centerInfo
getProperty chainInfo (atom expression)
getProperty dataInfo type
getProperty extractModel (atom expression)
getProperty fileContents
getProperty fileContents filepath
getProperty fileHeader
getProperty fileName
getProperty image
getProperty jmolStatus statusNameList
getProperty jmolViewer
getProperty measurementInfo
getProperty messageQueue
getProperty modelInfo
getProperty moleculeInfo (atom expression)
getProperty orientationInfo
getProperty polymerInfo (atom expression)
getProperty shapeInfo
getProperty stateInfo (atom expression)
getProperty transformInfo

halos ON/OFF{default: ON}
halos [radius-in-angstroms]
halos nn%

hbonds ON/OFF{default: ON}
hbonds [width-in-angstroms]
hbonds CALCULATE

help query

hide [atom-expression]

history ON/OFF{default: ON}

hover (integer)

initialize

invertSelected
invertSelected POINT point_definition
invertSelected PLANE plane_express
invertSelected HKL {h k l}

isosurface
isosurface DELETE
isosurface LIST

javascript "javascript commands"

label ON/OFF/string
label TOGGLE (atom expression)

lcaoCartoon ON/OFF{default: ON}
lcaoCartoon CREATE "[type]"
lcaoCartoon CREATE "[type]" MOLECULAR
lcaoCartoon COLOR [RGB-color]
lcaoCartoon COLOR [RGB-color] [RGB-color]
lcaoCartoon DELETE
lcaoCartoon LIST
lcaoCartoon ROTATE [x|y|z] (decimal) "[type]"
lcaoCartoon SCALE (decimal)
```

```
lcaoCartoon SELECT (atom expression)
lcaoCartoon SELECT "[type]"
lcaoCartoon TRANSLUCENT or OPAQUE

load
load "filename"
load [param-ignored] "filename"
load APPEND "filename"
load FILES "filename1" "filename2"
load "filename" (integer)
load "filename" {i j k}
load "filename" {ijk i'j'k' 1}
load "filename" {ijk i'j'k' 0}
load "filename" {ijk i'j'k' [0 or 1]} range xxx
load "" {i j k}
load "filename" {i j k} spacegroup "name"
load "filename" {i j k} spacegroup "ignoreOperators"
load "filename" {i j k} spacegroup "x,y,z;x+1/2,y,z"
load "filename" {i j k} unitcell {a b c alpha
    beta gamma}

loop [time-delay]
loop on

measure or monitor
measure ON/OFF{default: ON}
measure "n:labelFormat"
measure (integer) (integer) "labelFormat"
measure (integer) (integer) (integer) "labelFormat"
measure (integer) (integer) (integer)
    (integer) "labelFormat"
measure (two to four atom expressions, each in
    parentheses) labelFormat
measure ALL (two to four atom expressions, each
    in parentheses) "labelFormat"
measure ALLCONNECTED (two to four atom expressions,
    each in parentheses) "labelFormat"
measure DELETE
measure DELETE (integer)
measure DELETE (two to four atom expressions, each
    in parentheses)
measure RANGE (decimal) (decimal)
    ALL|ALLCONNECTED|DELETE

meshribbon ON/OFF{default: ON}
meshribbon [mesh-ribbon-radius]

message (string)

mo ON/OFF{default: ON}
mo (integer)
mo COLOR [RGB-color]
mo COLOR [RGB-color] [RGB-color]
mo CUTOFF (decimal)
mo DELETE
mo HOMO [+/-n]
mo LUMO [+/-n]
mo NEXT
mo NOPLANE
mo PLANE plane_expression
mo PREVIOUS [RGB-color]
mo RESOLUTION (decimal)
mo TITLEFORMAT "format"

model

move [x-rotation] [y-rotation] [z-rotation]
    [zoom-factor] [x-translation] [y-translation]
    [z-translation] [slab-cutoff] [seconds-total]
    [move-frames-per-second]{default: 30}
    [maximum-acceleration]{default: 5}

moveto timeSeconds FRONT|BACK|LEFT|RIGHT|TOP|BOTTOM
moveto timeSeconds {x y z} degrees zoomPercent transX
    transY {x y z} rotationRadius navigationCenter
    navTransX navTransY navDepth
moveto timeSeconds {x y z} degrees 0 transX transY
    (atom expression) 0 zoomAdjustment
    navigationCenter navTransX navTransY navDepth
moveto timeSeconds {x y z} degrees (atom expression)
    0 zoomAdjustment navigationCenter navTransX
    navTransY navDepth

navigate timeSeconds CENTER {x y z}
navigate timeSeconds CENTER (atom expression)
navigate timeSeconds CENTER $object
navigate timeSeconds DEPTH percent
navigate timeSeconds PATH $object
navigate timeSeconds PATH (any combination of
    coordinates, atom expressions, and objects)
navigate timeSeconds ROTATE X degrees
navigate timeSeconds ROTATE Y degrees
navigate timeSeconds ROTATE Z degrees
navigate timeSeconds TRACE (atom expression)
navigate timeSeconds TRANSLATE xxx yyy
navigate timeSeconds TRANSLATE X xxx
navigate timeSeconds TRANSLATE Y yyy
navigate timeSeconds TRANSLATE {x y z}
navigate timeSeconds TRANSLATE (atom expression)
navigate timeSeconds TRANSLATE $object

pause or wait

pmesh pmeshID{default: all pmeshes}
pmesh pmeshID{default: all pmeshes} ON/OFF{default: ON}
pmesh pmeshID{default: all pmeshes} DELETE
pmesh pmeshID(optional) "filename"
pmesh pmeshID{default: all pmeshes} DOTS or NODOTS
    {default: NODOTS} "xyz.pmesh.gz"{default: current}
pmesh pmeshID{default: all pmeshes} FILL or NOFILL
    {default: FILL} "xyz.pmesh.gz"{default: current}
pmesh LIST
pmesh pmeshID{default: all pmeshes} MESH or NOMESH
    {default: NOMESH} "xyz.pmesh.gz"{default: current}

polyhedra

ramachandran

refresh

reset AUTOMATIC
reset FUNCTIONS
reset variableName
reset ALL

restore BONDS saveName
restore ORIENTATION saveName timeSeconds
restore SELECTION saveName
restore STATE saveName

restrict {default: ALL}
restrict [atom-expression]

ribbon ON/OFF{default: ON}
ribbon [ribbon-radius]

rocket ON/OFF{default: ON}
rocket [rocket-radius]

rotate
rotate X/Y/Z [number-of-degrees]
```

```
rotate AXISANGLE [xyz-coordinate] [number-of-degrees]

rotateSelected

save
save BONDS saveName
save ORIENTATION saveName
save SELECTION saveName
save STATE saveName

script [file-name]
script [file-name] CHECK
script [file-name] COMMAND n
script [file-name] LINE n
script INLINE [Jmol math expression]
script INLINE varName
script javascript:functionCall()

select
select {default: ALL}
select [atom-expression]

selectionHalos
selectionHalos ON/OFF{default: ON}

set
set xxx?

set (antialiasing)
set antialiasDisplay OFF
set antialiasTranslucent ON
set antialiasImages ON

set (bond styles)
set bondMode AND
set bondMode OR
set bondModeOr FALSE
set bondRadiusMilliAngstroms (integer)
set bondTolerance (decimal)
set dipoleScale (-10.0 to 10.0)
set hbondsSolid FALSE
set hbondsBackbone FALSE
set minBondDistance (decimal)
set showMultipleBonds ON
set ssbonds BACKBONE or SIDECHAIN
set ssBondsBackbone FALSE

set (callback)
set AnimFrameCallback "function name"
set HoverCallback "function name"
set LoadStructCallback "function name"
set MessageCallback "function name"
set PickCallback "function name"
set ResizeCallback "function name"

set (debugging)
set debugScript OFF
set historyLevel (integer)
set logLevel (0 - 5)
set scriptReportingLevel (integer)
set showScript OFF
set showScript milliseconds

set (ellipsoids)
set ellipsoidAxes ON
set ellipsoidArcs ON
set ellipsoidBall ON
set ellipsoidFill ON

set (files and scripts)
set allowEmbeddedScripts
set appendNew TRUE
set appletProxy "URL"
set applySymmetryToBonds OFF
set autobond ON
set dataSeparator "separator text"
set defaultDirectory "directory path"
set defaultLattice {i j k}
set defaultLoadScript "script"
set forceAutoBond OFF
set history nLines
set loadFormat "URL"
set scriptQueue ON

set (highlights)
set display SELECTED/NORMAL
set fontSize [font-size]{default: 8}
set frank

set (labels)
set labelAlignment LEFT, RIGHT, or CENTER
set labelAtom (atom expression)
set labelFront (atom expression)
set labelGroup (atom expression)
set labelOffset [x-offset] [y-offset] (atom expression)
set labelPointer OFF (atom expression)
set labelPointer BACKGROUND (atom expression)
set labelToggle (atom expression)

set (language)

set (lighting)
set ambientPercent (integer 0 to 100)
set diffusePercent (integer 0 to 100)
set specular OFF
set specularExponent (integer 1 to 10)
set specularPercent (integer 0 to 100)
set specularPower (integer 0 to 100)

set (measure)
set defaultDistanceLabel "format"
set defaultAngleLabel "format"
set defaultTorsionLabel "format"
set dynamicMeasurements ON
set measurements [width-in-angstroms]
set measurements [linewidth-pixels]
set justifyMeasurements FALSE
set measurements DOTTED
set measurementLabels ON
set measurementUnits [distance-unit]
set showMeasurements TRUE

set (misc)
set allowRotateSelected FALSE
set animationFps (integer)
set autoFPS FALSE
set axis1Color "color_name"
set axis2Color "color_name"
set axis3Color "color_name"
set backgroundModel (integer >= 1) or "filemodel"
set chainCaseSensitive FALSE
set colorRasmol FALSE
set defaultColorScheme JMOL or RASMOL
set defaultDrawArrowScale (decimal)
set defaults JMOL or RASMOL
set dotsSelectedOnly FALSE
set dotSurface ON
set drawHover OFF
set drawPicking OFF
set exportDrivers "driver_list"
set formalCharge (integer)
set helpPath "URL"
```

```
set hoverDelay (decimal)
set hoverLabel (string)
set isosurfacePropertySmoothing ON
set measureAllModels OFF
set percentVdwAtom (integer)
set pickingSpinRate (integer)
set propertyAtomNumberField (integer)
set propertyColorScheme "colorSchemeName"
set propertyDataField (integer)
set rangeSelected
set selectHetero ON
set selectHydrogen ON
set smartAromatic ON
set spinFps [frames-per-second]
set spinX [degrees-per-second]
set spinY [degrees-per-second]
set spinZ [degrees-per-second]
set stateVersion (integer)
set statusReporting ON
set stereoDegrees (decimal)
set syncMouse OFF
set syncScript OFF
set useNumberLocalization ON
set vectorScale (decimal)
set vibrationPeriod (decimal)
set vibrationScale (decimal)
set wireframeRotation OFF

set (navigation)
set hideNavigationPoint FALSE
set navigationDepth (percent)
set navigationMode FALSE
set navigationPeriodic FALSE
set navigationSpeed (decimal)
set navigationSlab (percent)
set showNavigationPointAlways FALSE
set visualRange (angstroms)

set (perspective)
set cameraDepth (positive number)
set perspectiveDepth ON
set perspectiveModel 11
set scaleAngstromsPerInch [viewing-distance]
set rotationRadius (Angstroms)
set windowCentered ON
set zoomEnabled ON
set zoomLarge ON
set zShade OFF

set (structure)
set cartoonRockets OFF
set hermiteLevel (integer, -8 to 8)
set highResolution OFF
set ribbonAspectRatio (integer)
set ribbonBorder OFF
set rocketBarrels OFF
set sheetSmoothing (0 to 1)
set strandCount [strand-count]
set strandCountForMeshRibbon [strand-count]
set strandCountForStrands [strand-count]
set traceAlpha TRUE

set (visibility)
set axes [line-width-or-type]
set axesMode 0, 1, or 2
set axesMolecular OFF
set axesScale (decimal)
set axesUnitcell OFF
set axesWindow ON
set backgroundColor [RGB-color]
set boundbox [line-width-or-type]
set defaultTranslucent (decimal)
set disablePopupMenu FALSE
set displayCellParameters TRUE
set greyScaleRendering OFF
set hideNameInPopUp FALSE
set hideNotSelected FALSE
set refreshing TRUE
set showAxes FALSE
set showBoundBox FALSE
set showFrank TRUE
set showHiddenSelectionHalos FALSE
set showHydrogens TRUE
set showSelections FALSE
set showUnitcell FALSE
set slabEnabled FALSE
set solventProbe OFF
set solventProbeRadius [probe-radius-in-angstroms]
    {default: 1.2}
set unitcell

set echo
set echo user-named [horizontal-position]
    {default: left}
set echo user-named x-position y-position
set echo user-named %x %y
set echo user-named {x y z}
set echo user-named { [atom-expression] }}
set echo [vertical-position] ON
set echo user-named ON
set echo ALL
set echo NONE
set echo OFF

set picking
set picking ON
set picking CENTER
set picking DRAW
set picking IDENT
set picking LABEL
set picking MEASURE
set picking MEASURE DISTANCE
set picking MEASURE ANGLE
set picking MEASURE TORSION
set picking NAVIGATION
set picking SELECT ATOM
set picking SELECT CHAIN
set picking SELECT ELEMENT
set picking SELECT GROUP
set picking SELECT MOLECULE
set picking SELECT SITE
set picking SPIN [frames-per-second]

set pickingStyle
set pickingStyle SELECT toggle
set pickingStyle SELECT selectOrToggle
set pickingStyle SELECT extendedSelect
set pickingStyle SELECT NONE
set pickingStyle MEASURE ON

set userColorScheme
set userColorScheme colorName colorName

show BOUNDBOX
show CENTER
show COLORSCHEME "name"
show DATA "type"
show DRAW
show FILE
show FILE filepath
show ISOSURFACE
show FUNCTIONS
```

```
show HISTORY n
show MEASUREMENTS
show MO
show MODEL
show ORIENTATION
show PDBHEADER
show SET
show SPACEGROUP "name"
show STATE [optional name]
show SYMMETRY
show TRANSFORM
show UNITCELL
show URL
show URL URL
show ZOOM
show $objectID

slab ON/OFF{default: ON}
slab [slab-percent]
slab HKL {h k l} or NONE
slab -HKL {h k l}
slab PLANE plane_expression or NONE
slab -PLANE plane_expression
slab RESET
slab SET

spacefill ON/OFF{default: ON}
spacefill [radius-in-angstroms]
spacefill [radius-percent-vdw]
spacefill +(solvent probe radius)
spacefill IONIC
spacefill TEMPERATURE

spin
spin ON/OFF{default: ON}

ssbonds ON/OFF{default: ON}
ssbonds [width-angstroms]
ssbonds [width-Rasmol]

star ON/OFF{default: ON}
star [length-in-angstroms]
star nn%

stereo [stereo-viewing-angle]{default: 5}
stereo {default: ON}
stereo OFF
stereo REDBLUE [stereo-viewing-angle]{default: 3}
stereo REDCYAN [stereo-viewing-angle]{default: 3}
stereo REDGREEN [stereo-viewing-angle]{default: 3}
stereo [RGB-color] [RGB-color] [stereo-viewing-angle]
    {default: 3}

strands ON/OFF{default: ON}
strands [strand-radius]

subset

sync &PER;|>|*|appletId|appletId[syncId] ON
sync &PER;|>|*|appletId|appletId[syncId] SLAVE
sync &PER;|>|*|appletId|appletId[syncId] OFF
sync &PER;|>|*|appletId|appletId[syncId] "command"

trace ON/OFF{default: ON}
trace [trace-radius]

translate
translate X or Y [percent-translation]

translateSelected
translateSelected {x y z}

unitcell ON/OFF{default: ON}
unitcell (decimal)
unitcell DOTTED
unitcell {i j k}

vector ON/OFF{default: ON}
vector [diameter-pixels]
vector [radius-in-angstroms]
vector SCALE [vector-scale]

vibration ON/OFF{default: ON}
vibration [time-period]
vibration PERIOD [time-period]
vibration SCALE [vibration-scale]

wireframe ON/OFF{default: ON}
wireframe [radius-in-angstroms]
wireframe [radius-Rasmol]

write
write fileName
write COORDS SPT|XYZ|MOL|PDB "fileName"
write FILE "fileName"
write FUNCTIONS "fileName"
write HISTORY "fileName"
write IMAGE JPG|JPG64 n "fileName"
write IMAGE PNG n "fileName"
write IMAGE PPM "fileName"
write ISOSURFACE "fileName"
write MO "fileName"
write STATE "fileName"
write VAR [variable name] "fileName"

zap

zoom ON/OFF{default: ON}
zoom [percent-zoom]
zoom (atom expression) or {x y z} [percent-zoom]
zoom (atom expression) or {x y z} + or - delta
zoom (atom expression) or {x y z} * or / factor

zoomto
zoomto OUT
zoomto [time-in-seconds] (atom expression) or {x y z}
zoomto [time-in-seconds] (atom expression) or {x y z}
    [percent-zoom]
zoomto [time-in-seconds] (atom expression) or {x y z}
    + or - delta
zoomto [time-in-seconds] (atom expression) or {x y z}
    * or / factor
zoomto [time-in-seconds] (atom expression) or {x y z} 0
```