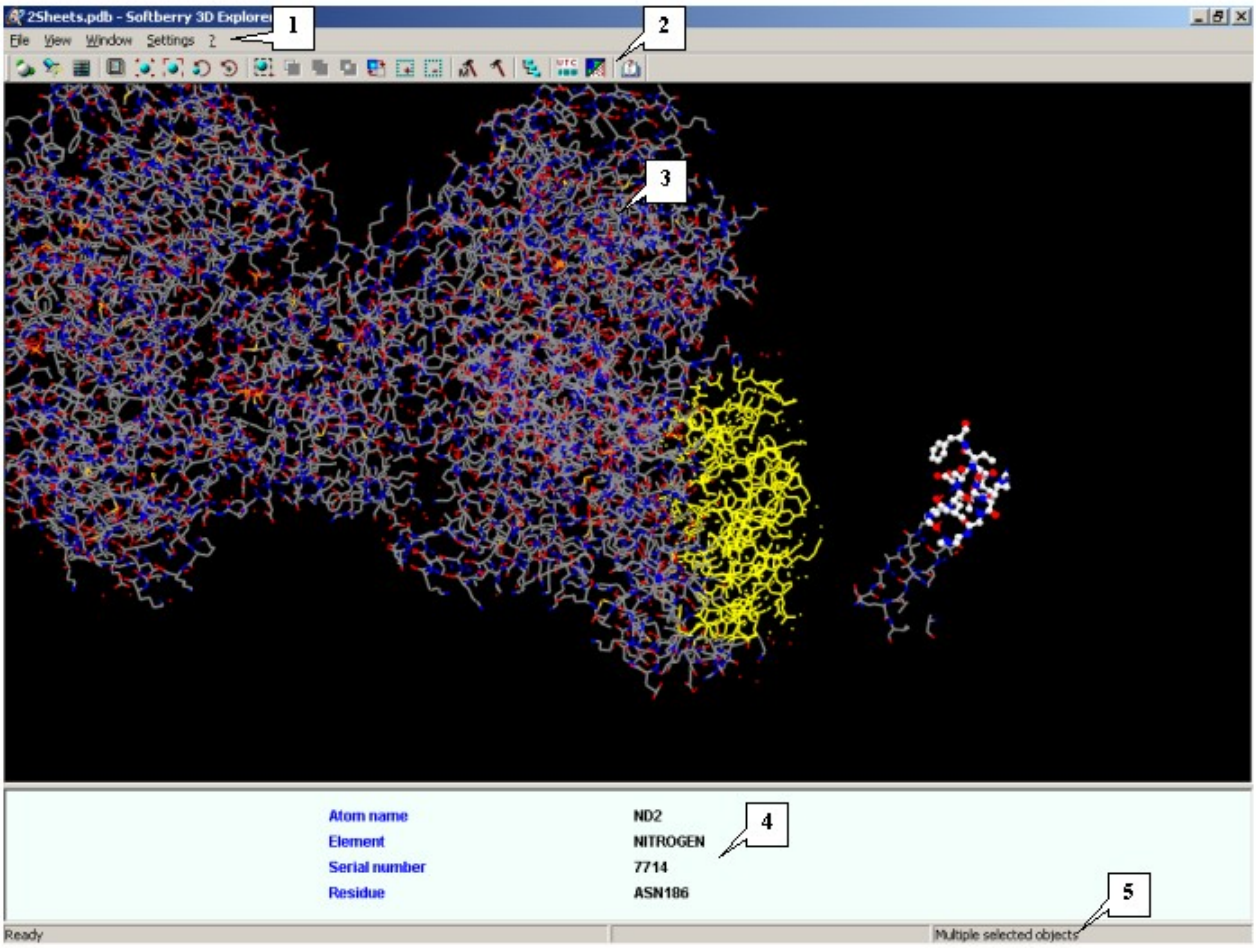
Contents

Introduction

3D Explorer is designed to visualize spatial models of biological macromolecules and their complexes (below referred to as models). The **3D**

Explorer application is compatible with PDB files [1].
3D Explorer has an interface compatible with the GetAtoms and CE applications [2, 3].
The macromolecule can be presented as wire, stick, ball and stick, and CPK models.
You can drag a macromolecule model with your mouse, rotate it, and change the size of models.
You can also change the detail level and color of models and their elements.
In **3D Explorer**, you can work with several types of molecular elements and show the structural features of a molecule as a matrix diagram.

Application window



1. Main menu. **2.** Toolbar. **3.** View area. **4.** Information panel. **5.** Status bar.

Main menu commands

The **File** menu contains the commands for loading and adding model to the scene:

- **Open** - Load a model.

- **Add** - Add a model to the scene.

The **View** menu has the commands for customizing the model view:

- **Detail level** - Select the following detail levels for the model:
  - **Very low**
  - **Low**
  - **Normal**
  - **High**
  - **Very high**
- **Animation** - Configure the automatic rotation of the model:
  - **Spin** - enable (disable) the rotation of the model.
  - **Set delay** - Display the **Set delay** dialog where you can set the delay for model rotation.
- **Display** - Open the **Display options** dialog to customize the geometry and color settings for the model.
- **Light options** - Open the **Light options** dialog to customize settings for lighting the model.
- **Colors** - Open the **Color dialog** to select colors for particular chemical elements.
- **Model options** - Open the **Model Options** dialog to select the types of atoms, chains, aminoacid residues, and chemical elements to be displayed in the model.
- **Options** - Open the **Options** dialog to customize the general view of the model and mouse settings.
- **Fullscreen** - Display the view area in full-screen mode.

The **Window** menu has the commands for open viewers and diagram:

- **Tree dialog** - Display the **Tree explorer** dialog to view the hierarchical structure of the molecular elements.
- **Sequence viewer** - Open the **Sequence viewer** dialog to display sequences of protein chains.
- **Matrix dialog** - Open the **Matrix diagram** dialog to display specific features of the molecular structure as a matrix diagram.

The **Settings** menu contains**:**

- **Save settings** - Saves the basic options of the application. The kept options will be restored at following start of the application.

The **?** menu has the help commands:

- **Help** - Refer to Help Topics.
- **About** - Open the "About" dialog.

Toolbar

Functions of Toolbar buttons:

	**Display options** - Open the **Display options** dialog to customize the geometry and color settings for the model. Does the same as: **View>Display** in the Main Menu.
	**Light options** - Open the **Light options** dialog to customize settings for lighting the model. Does the same as: **View>Light options** in the Main Menu.
	**Color options** - Open the **Color dialog** to select colors for specific chemical elements. Does the same as: **View>Colors** in the Main Menu.
	**Full screen** - Display the view area in full-screen mode. Does the same as:**View>Fullscreen** in the Main Menu.
	**Reset model position** - Resets the initial model position.
	**Fit to window** - Change the model size to fit the view area.
	**Select rotation center mode** - When this mode is enabled, the user can assign an atom to be the rotation center for the entire model.
	**Reset rotation center** - Reset the rotation center at the geometrical center of the model.
	To turn on the **«transformation» mode**. In this mode, the movement, rotation and changing of a distance operations can be performed for selected elements of scene only.
	**Select mode on/off** - Enable/disable selection mode.
	**Normal selection mode** - In normal selection mode, each subsequent selection unselects the previously selected item.
	**OR selection mode** - In OR selection mode, all subsequent selections are added to the previously selected items.
	**XOR selection mode** - In XOR selection mode, a previously selected item is unselected by subsequent selection.
	**Inverse selection** - Invert a selection.
	**Select all** - Select all elements of the model.
	**Unselect all** - Unselect all elements of the model.

	**Model options** - Open the **Model Options** dialog to select the types of atoms, chains, aminoacid residues, and chemical elements to be displayed by the program. Does the same as: **View>Model options** in the Main Menu.
	**Options** - Open the **Options** dialog to customize the general view of the model and mouse settings. Does the same as: **View>Options** in the Main Menu.
	**Tree model dialog** - Open the **Tree explorer dialog** to view the hierarchical structure of the model elements. Does the same as: **Window>Tree dialog** in the Main Menu.
	**Sequence viewer** - Open the **Sequence viewer** dialog to display sequences of protein chains. Does the same as: **Window>Sequenc** in the Main Menu.
	**Matrix viewer** - Open the **Matrix diagram** dialog to display specific features of the molecular structure as a matrix diagram. Does the same as: **Window>Matrix dialog** in the Main Menu.
	**Help** - Refer to Help Topics. Does the same as: **?>Help** in the Main Menu.

Note. Place your mouse pointer over a toolbar button to see the function of this button in the status bar.

View area

The view area displays models in the user-defined view mode. In the view area, you can change the distance to the model, move and rotate models, and select fragments of the model. Dashed lines indicate hydrogen bonds.
Use the **Options** dialog to change the background color of the view area.
You can move the border between the view area and the information panel by dragging it with your mouse.

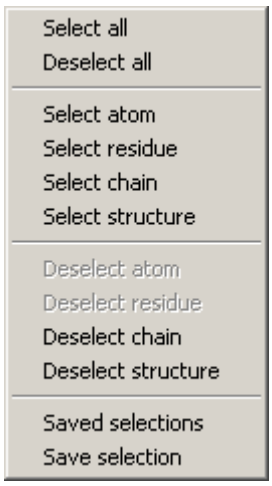
Shortcut menu

To open a shortcut menu, right-click the view area.

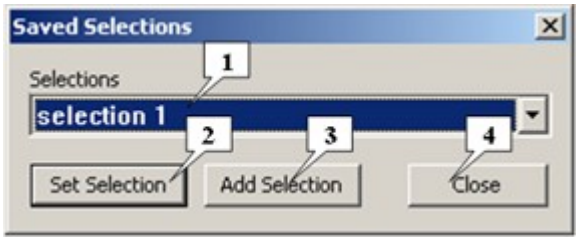
The shortcut menu includes the following items:

- **Select all** - Select all models.
- **Deselect all** - Deselect all models.
- **Select atom** - Select the atom you are pointing to with your mouse.
- **Select residue** - Select the residue you are pointing to with your mouse.
- **Select chain** - Select the chain you are pointing to with your mouse.
- **Select structure** - Select the model you are pointing to with your mouse.
- **Deselect atom** - Deselect an atom.
- **Deselect residue** - Deselect a residue.
- **Deselect chain** - Deselect a chain.

View area shortcut menu

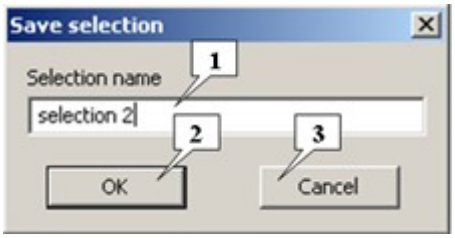


- **Deselect structure** - Deselect a model.
- **Saved selections** - opens the **Saved Selections** dialog, purposed for choosing of saved selections. A selection must be chosen from the list. The **Set selection** button is used for changing of the current scene's selection to a chosen one. The **Add selection** button is used for adding of the chosen selection to the current selection of the scene's elements.



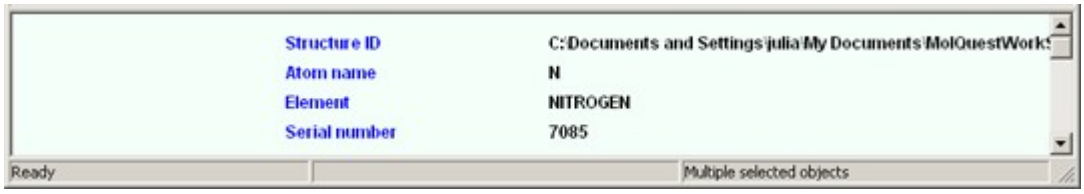
1. The list of saved selections. **2.** Button for changing of the current scene's selection to a chosen one. **3.** Button for adding of the chosen selection to the already present in the scene ones. **4.** Button for closing of the dialog.

- **Save selection** - opens the **Save selection** dialog, purposed for saving of the current selection. It requires to enter the name of selection and press the **OK** button.



1. The selection's name entry field. **2.** Button for saving of the selection and closing of the dialog. **3.** Button for canceling of the selection's saving and closing of the dialog.

Information panel



The information panel displays:

- Information about the atom you are pointing to with your mouse: atom name, chemical element, number of the atom in the PDB file, and the name of the residue this atom belongs to.
- Information about the residue you are pointing to with your mouse: residue name, chain identifier, type of the secondary structure, indices of N- and C-terminal residues for the secondary structure this residue belongs to.

Status bar

The status bar displays:

- The function of the toolbar button you are pointing to with your mouse;
- Selection status.

Loading a model

Loading a file

To load a model, click **File>Open**. In the dialog that appears on your screen, select the file to be loaded. All previously loaded models are deleted from the scene.

Adding a model

To add a model to the existing ones, click **File>Add**. In the dialog that appears on your screen, select the file to be added.

Working with images

Customizing image parameters

Adjusting image quality

To change the image quality, do one of the following:

- Click **View>Detail level** in the main menu and select one of the following options:

    - **Very low**
    - **Low**
    - **Normal**
    - **High**
    - **Very high**
- Change the Detail level parameter in the **Options** dialog.

Customizing the view

To open the **Display options** dialog, click:

- **View>Display style** in the main menu.
- The  toolbar button.

The **Display options** dialog has two tabs: **Geometry** and **Sizes**. If any of the scene elements are selected, changes will be applied only to the selected elements. If no elements are selected, changes will be applied to all the scene elements.

***Geometry* tab**

The **Geometry** tab is used to specify the types of geometry for the elements of the model.

The **Group** column contains the names of groups with adjustable viewing parameters:

- **Protein backbone** - Protein backbones
- **Protein sidechain** - Aminoacid residue side groups
- **Nucleotide backbone** - DNA sugar-phosphate backbone
- **Nucleotide base** - DNA nucleotide bases
- **Solvent** - Solvent atoms
- **Heterogene** - Heteroatoms
- **Protein structure** - A schematic representation of the protein backbone.

For the Protein backbone group, the following options are available in the drop-and-down lists of the**Modes** column:

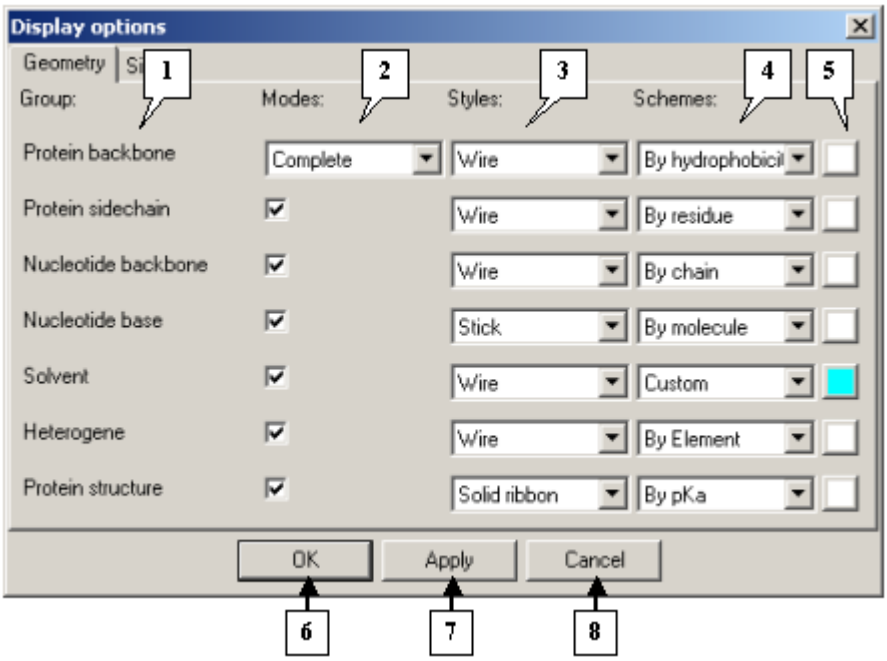
- **Complete** - Display all protein backbone atoms: Cα, N, C, and O.
- **Partial** - Display only some protein backbone atoms: Cα, N, and C.
- **Trace** - Display only Cα atoms in the protein backbone.
- **None** - Hide protein backbones.

The **Styles** column has the following options for the Protein backbone, Protein sidechain, Nucleotide backbone, Nucleotide base, Solvent, and Heterogene groups:

- **Wire** - A wire (skeleton) model. Atomic bonds are shown with lines.

- **Ball and Stick** - A "ball and stick" model. Atoms are shown as spheres and atomic bonds, as sticks. The stick radius is set in the **Stick size** field and the sphere radius, in the **Ball size** field on the **Atoms** pane of the **Sizes** tab.
- **Stick** - A stick model. Atomic bonds are shown as sticks. The stick radius is set in the **Stick size**field on the **Atoms** pane of the **Sizes** tab.
- **CPK** - A full atomic model (space-filling). The sphere radii are proportional to van der Waals atomic radii. The sphere scale is defined in the **CPK scale** field on the **Atoms pane** of the **Sizes**tab.

The *The Display options* dialog. The *Geometry* tab



1. Group names. **2.** Viewing modes. **3.** Drop-and-down lists for selecting viewing styles. **4.** Drop-and-down lists for selecting color schemes. **5.** Buttons for selecting colors in **Custom** mode. **6.**The **OK** button applies changes and closes the dialog. **7.** The **Apply** button applies changes and leaves the dialog open. **8.** The **Cancel** button closes the dialog and cancels changes.

The **Styles** list for the **Protein structure** group contains the following options:

- **Wire ribbon** - Show a protein backbone as a thin ribbon.
- **Flat ribbon** - Show a protein backbone as a flat ribbon.
- **Solid ribbon** - Show a protein backbone as a solid ribbon. The ribbon width can be changed in the **Ribbon width** field of the **Ribbons** pane on the **Sizes** tab.
- **Wire schematic** - Show a central line of the elements displayed in the Solid schematic view.
- **Solid schematic** - Show schematically the secondary protein structure: α-helixes are displayed as wide sticks, β-sheets, as arrows, and transitions, turns, and unknown structures, as narrow sticks. The arrow width is set in the **Strand width** field and the radius of the sticks showing α-helixes, in the **Helix radius** field on the **Schematic** pane of the **Sizes** tab.

- **Wire trace** - Display traces connecting the Cα atoms of the backbone.
- **Solid trace** - Show sticks connecting the Cα-atoms of the backbone. The stick radius is set in the **Trace radius** field on the **Trace** pane of the **Sizes** tab.
- **Wire worm** - Display the backbone as a thin line.
- **Solid worm** - Display the backbone as a thin pipe. The pipe radius is set in the **Worm radius**field of the **Trace** pane on the **Sizes** tab.

The **Schemes** list contains the following options:

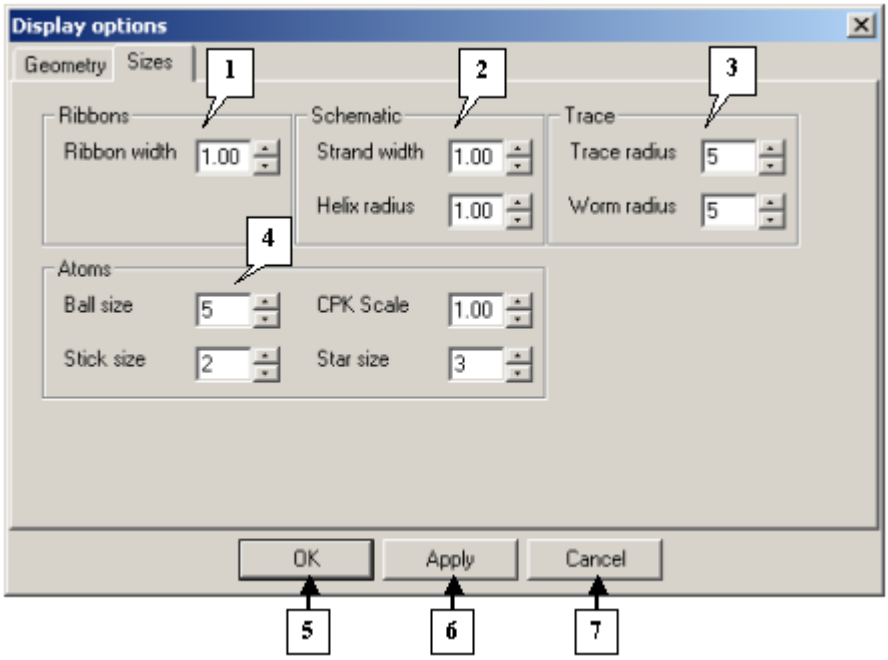
- **By Element** - the color of an atom is determined by the color of its chemical element (the colors of chemical elements are set in the **Color dialog**.
- **By Residue** - the color of an element of the model is determined by the residue it belongs to. In this case, the residue is any group of covalently bound atoms (aminoacids, nucleotides, and heterogroups).
- **By Chain** - the color of an element of the model is determined by the chain it belongs to.
- **By molecule** - the color of an element of the model is determined by the model it belongs to.
- **By hydrophobicity** - the color of elements in a group is determined by hydrophobic properties of the aminoacid it belongs to.
- **By pKa** - the color of elements in a group depends on the pKa constant of the aminoacid it belongs to.
- **By Secondary structure** - the color of elements in a group depends on the secondary structure of a chain fragment. α-helixes are red, β-structures are blue, and turns and non-structured fragments are white.
- **By alignment** - the color of elements in a group depends on the alignment pattern. Aligned fragments in sequences are red and non-aligned fragments are white.
- **Custom** - the color of a group is defined by user. Click the ▭ button to open the **Color** dialog where you can select a color.

Notes:
For the Protein backbone and Protein sidechain groups, the Schemes list contains all available modes.
For the Nucleotide backbone, Nucleotide base, Solvent, and Heterogene groups, the **Schemes** list contains only the **By Element**, **By Residue**, **By Chain**, **By molecule**, and **Custom** modes.
For the Protein structure group, the **Schemes** list contains all modes except for **By Element**.

Sizes tab

On the **Sizes** tab you can change the geometrical parameters of models.

The *Display options* dialog. The *Sizes* tab



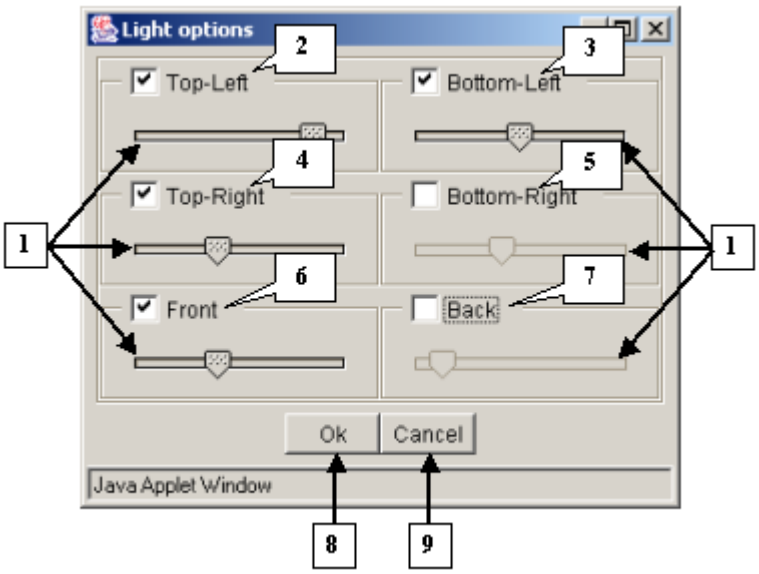
1. The **Ribbons** pane. **2.** The **Schematic** pane. **3.** The **Trace** pane. **4.** The **Atoms** pane. **5.** The**OK** button applies changes and closes the dialog. **6.** The **Apply** button applies changes and leaves the dialog open. **7.** The **Cancel** button closes the dialog and cancels changes.

- The **Ribbons** pane is used to customize the viewing parameters of the **Wire ribbon**, **Flat ribbon**, and **Solid ribbon** styles.
  - In the **Ribbon width** field, click the up and down arrows to specify the ribbon width.
- The **Schematic** pane is used to change the viewing parameters of the **Solid schematic** style.
  - In the **Strand** width field, adjust the width of the arrows showing β-sheets.
  - In the **Helix** radius field, change the radius of the sticks denoting α-helixes.
- The **Trace** pane is designed to change the viewing parameters of the **Solid trace** and **Solid worm** styles.
  - In the **Trace radius** field, change the radius of the trace in the **Solid trace** style.
  - In the **Worm radius** field, customize the radius of the thin pipe in the **Solid worm** style.
- The **Atoms** pane is used to change the following viewing parameters for atoms:
  - In the **Ball size** field, change the ball radius for the **Ball and Stick** style.
  - In the **Stick size** field, change the stick radius for the **Ball and Stick** style.
  - In the **CPK Scale**, customize the scale of spheres for the **CPK** style.

- In the **Star size** field, adjust the size of stars showing standalone atoms (without bonds).

Light options

The *Light options* dialog



1. Sliders. **2.** Upper left source. **3.** Lower left source. **4.** Upper right source. **5.** Lower right source.**6.** Front source. **7.** Background source. **8.** The **OK** button applies changes and closes the dialog. **9.**The **Cancel** button closes the dialog and cancels changes.

To open the **Light options** dialog, do one of the following:

- Select **View>Light** options in the main menu.
- Click the  toolbar button

3D-Explorer allows the user to choose between six light sources that can be selected by checking the corresponding boxes:

- **Top-Left** - the light source is placed on the left above the model.
- **Bottom-Left** - the light source is placed on the left below the model.
- **Top-Right** - the light source is placed on the right above the model.
- **Bottom-Right** - the light source is placed on the right below the model.
- **Front** - the light source is placed in front of the model.
- **Back** - the light source is placed behind the model.

Adjust the intensity of the light sources by moving the corresponding sliders.

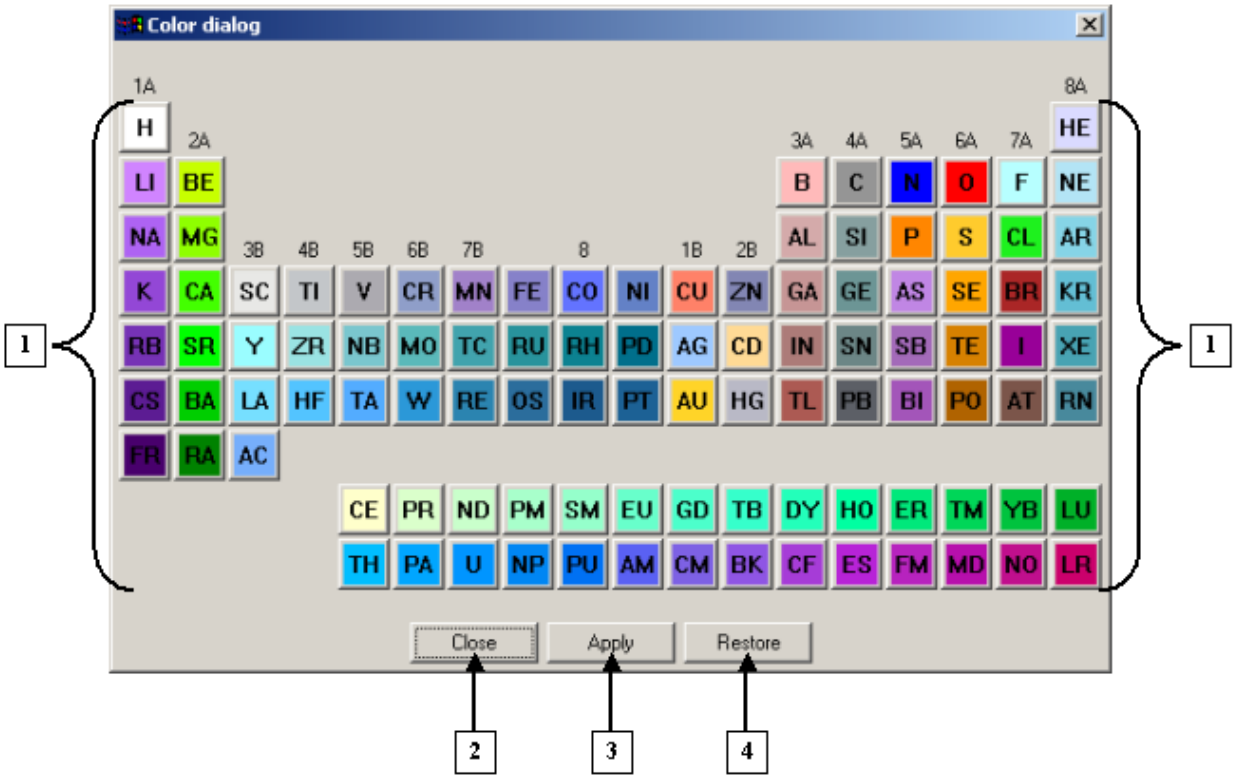
Selecting colors of chemical elements

You can change the colors of chemical elements in the **Color dialog**. To open this dialog:

- Select the **View>Colors** command in the main menu.

- Click the  toolbar button.

The *Color dialog*



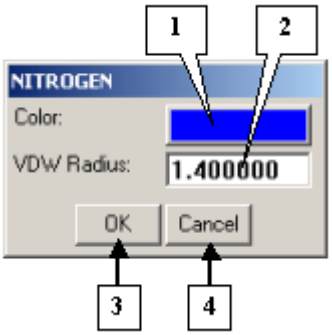
1. Buttons for changing the colors of chemical elements. **2.** The **Close** button. **3.** The **Apply** button. **4.** The**Restore** button.

The **Color dialog** contains colored buttons that are used to customize the colors of chemical elements. Each color corresponds to a certain element.

Click a colored button with the name of a chemical element to open a dialog for this specific element, for example, "NITROGEN":

- The **Color** button shows the current color of the element. After you click this button, the **Color** dialog will appear on your screen. In this dialog, change the color of a chemical element. The**Color** button will change its, too. Click **OK** to close the dialog and apply changes. In the **Color dialog**, the button with the name of the chemical element will be colored according to the changes you made.
- The **VDW Radius** field contains the default value of the van der Waals radius of a chemical element. This value can be changed by the user. If you click **OK** in this dialog and then click either the **Close** or **Apply** buttons in the **Color dialog** , the model will be changed according to the new parameters.

The *NITROGEN* dialog



1. The button for adjusting the color of the chemical element. **2.** The **VDW Radius** field for changing the default van der Waals radius of the element. **3.** The **OK** button applies changes and closes the dialog. **4.** The **Cancel** button closes the dialog and cancels changes.

***Color dialog* control buttons:**

- **Close** - Apply changes and close the dialog.
- **Apply** - Apply changes and leave the dialog open.
- **Restore** - Reset the default values of the van der Waals radii of the elements and default colors.

Model motions

- Moving the model
- Rotating the model
- Changing the distance to the model

Moving the model

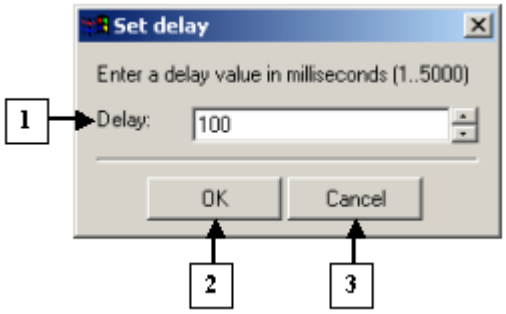
To move the model, drag the molecule image over the view area with your mouse while pressing the**Ctrl** key on your keyboard. If  button is pressed, only selected elements of the scene can be replaced.

Rotating the model

You can rotate the model using your mouse. The rotation speed is adjusted in the **Options** dialog. If  button is pressed, only selected elements of the scene can be rotated.

The automatic rotation of the model is disabled by clicking **View>Animation>Spin** in the main menu. You can customize the rotation speed by setting the rotation delay (in milliseconds) in the **Set delay**dialog. Select **View>Animation>Set delay** in the main menu to open this dialog. The automatic rotation of the model is available only in that case when there is no selected elements on the scene.

The *Set delay* dialog



1. The field for entering the delay value for shot changes. **2.** The **OK** button applies changes and closes the dialog. **3.** The **Cancel** button closes the dialog and cancels changes.

By default, the model turns around its geometrical center. You can change the geometrical center of the model. To set another geometrical center:

1. Enable the center selection mode by clicking the toolbar button. After this, the current geometrical center will be selected.
2. Click the atom you want to set as a geometrical center. The new geometrical center will be selected in the view area.
3. Disable the center selection mode by clicking the toolbar button.

Changing the distance to the model

You can change the distance to the model using your mouse while pressing the **Shift** key on your keyboard. If the mouse pointer is moving downwards, the model is zoomed out; if the mouse pointer is moving upwards, the model is zoomed in. The scaling speed is adjusted in the **Options** dialog. If button is pressed, a distance to selected elements of the scene only can be changed.

Notes.
To load the initial image of the model, click the toolbar button.
To make the model fit the view area, click the toolbar button.

Selecting elements of the model

- **Selection modes**
- **Shortcut menu**

Selection modes

You can select specific elements of the model by using your mouse. The selection mode is enabled by clicking the toolbar button.

When the toolbar button is switched on, the following buttons become available:
- **Normal selection mode** - In this mode, each subsequent selection unselects the previously selected item.
- **OR selection mode** - In this mode, all subsequent selections are added to the previously selected items.
- **XOR selection mode** - In this mode, a previously selected item is unselected by subsequent selection.

Click the toolbar button to invert a selection.

Click the toolbar button to select all elements in the model.

Click the toolbar button to unselect all elements of the model.

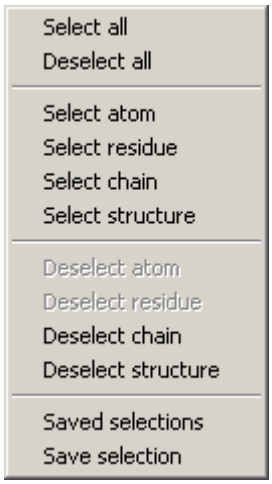
Note.
The elements of models can also be selected using the **Tree explorer** and **Sequence viewer** dialogs.

Shortcut menu

You can select specific elements of the model by using **Shortcut menu**.

To open a shortcut menu, right-click the view area.

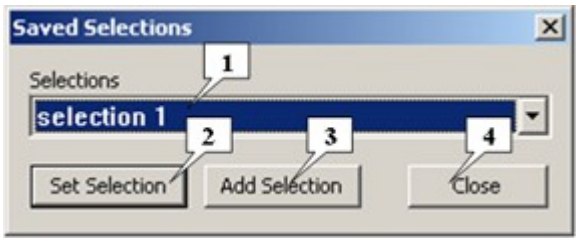
View area shortcut menu



The shortcut menu includes the following items:

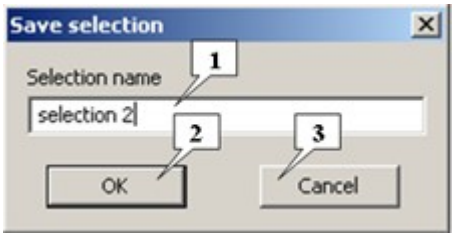
- **Select all** - Select all models.
- **Deselect all** - Deselect all models.
- **Select atom** - Select the atom you are pointing to with your mouse.
- **Select residue** - Select the residue you are pointing to with your mouse.
- **Select chain** - Select the chain you are pointing to with your mouse.
- **Select structure** - Select the model you are pointing to with your mouse.
- **Deselect atom** - Deselect an atom.

- **Deselect residue** - Deselect a residue.
- **Deselect chain** - Deselect a chain.
- **Deselect structure** - Deselect a model.
- **Saved selections** - opens the **Saved Selections** dialog, purposed for choosing of saved selections. A selection must be chosen from the list. The **Set selection** button is used for changing of the current scene's selection to a chosen one. The **Add selection** button is used for adding of the chosen selection to the current selection of the scene's elements.



1. The list of saved selections. **2.** Button for changing of the current scene's selection to a chosen one. **3.** Button for adding of the chosen selection to the already present in the scene ones. **4.** Button for closing of the dialog.

- **Save selection** - opens the **Save selection** dialog, purposed for saving of the current selection. It requires to enter the name of selection and press the **OK** button.



1. The selection's name entry field. **2.** Button for saving of the selection and closing of the dialog. **3.** Button for canceling of the selection's saving and closing of the dialog.

Lists of model elements

- Hierarchical tree
- Sequence viewer

Hierarchical tree

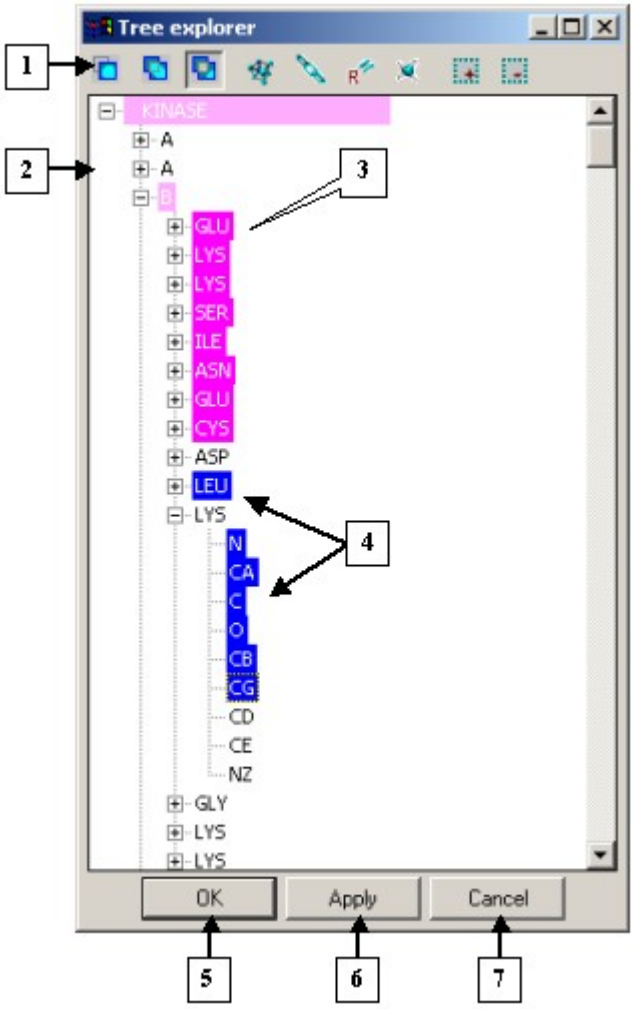
The **Tree explorer** dialog contains the hierarchical tree of the elements of a model that can be generated by:

- Selecting the **Window>Tree dialog** option in the main menu
- Clicking the  toolbar button.

The **Tree explorer** dialog contains the following elements:

- Control panel
- List of model elements
- Dialog control buttons

The *Tree explorer* dialog



1. Control panel. **2.** Tree of model elements. **3.** Selections applied. **4.** New selections. **5.** The **OK**button. **6.** The **Apply** button. **7.** The **Cancel** button.

Control panel buttons

 - Enable the normal selection mode in which each subsequent selection unselects the previously selected item. To select an item, click it with your mouse.

 - Enable the OR selection mode in which all subsequent selections are added to the previously selected items. To select an item, click it with your mouse.

 - Enable the XOR selection mode in which a previously selected item is unselected by subsequent selection. To select an item, click it with your mouse.

 - Expand the tree branch to the molecule level.

 - Expand the tree branch to the chain level.

 - Expand the tree branch to the residue level.

 - Expand the tree branch to the atom level.
 - Select all elements in the tree.
 - Unselect all elements in the tree.

Tree of model elements

The tree shows the hierarchical structure of model elements. You can select elements in the tree with your mouse. Change the selection modes by clicking the control panel buttons.

The selected items are highlighted in blue.

The elements with the applied selection are highlighted in pink.

Dialog control buttons

- Click **OK** to apply selections and close the dialog.
- Click **Apply** to apply selections and leave the dialog open.
- Click **Cancel** to close the dialog and cancel the current selections.

Sequence viewer dialog

You can open the **Sequence viewer** dialog designed to view sequences of protein chains by:

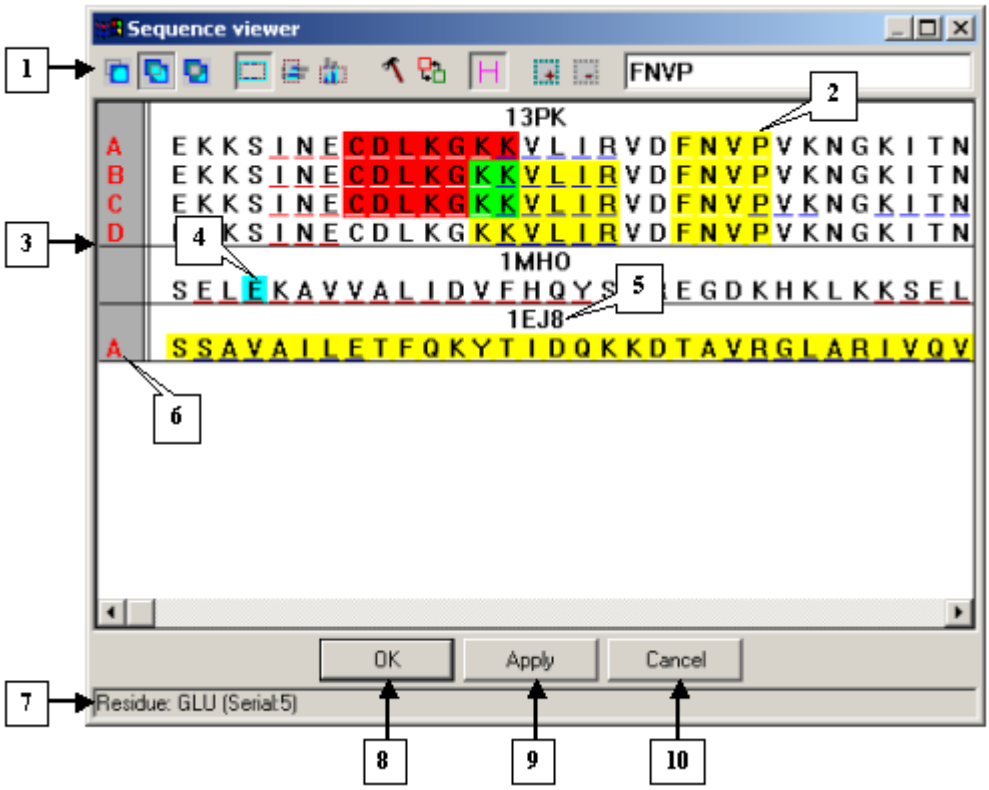
- Selecting the **Window>Sequence viewer** option in the main menu.
- Clicking the  toolbar button.

Structure of the *Sequence viewer* dialog

The **Sequence viewer** dialog contains:

- Control panel
- Sequence view area
- Dialog control buttons
- Status bar

The *Sequence viewer* dialog



1. Control panel. **2.** Search result. **3.** Sequence view area. **4.** Mouse cursor position in the sequence view area (the residue is highlighted in blue). **5.** Model name. **6.** Chain identifiers. **7.**Status bar. **8.** The **OK** button. **9.** The **Apply** button. **10.** The **Cancel** button.

Control panel

The control panel buttons have the following functions:

- **Normal selection mode**. In this mode, each subsequent selection unselects the previously selected item. To select an item, click it with your mouse or select a rectangular area with your mouse pointer.

- **OR selection mode**. In this mode, all subsequent selections are added to the previously selected items. To select an item, click it with your mouse or select a rectangular area with your mouse pointer.

- **XOR selection mode**. In this mode, a previously selected item is unselected by subsequent selection. To select an item, click it with your mouse or select a rectangular area with your mouse pointer.

- **Rectangle area selection mode**. In this mode, the program selects all residues within a rectangular area defined by the motion of your mouse.

- **Lines selection mode**. In this mode, the program selects all residues located in the rows you select by moving your mouse.

- **Columns selection mode**. In this mode, the program selects all residues located in the columns you select by moving your mouse.

- **Options**. Click this button to open the **Options** dialog of the Sequence viewer dialog.

 - **Hide or show elements**. Click this button to open the **Visible and hidden elements** dialog in which you can enable/disable some models to be displayed in the sequence view area.
 - **Hide or show headers of elements**. In this mode, model names are shown above chain sequences.
 - **Select all**. Select all elements in the list.
 - **Deselect all**. Deselect all elements in the list.

In the upper right corner of the dialog there is an input field used to search for specified fragments (templates) in chains. Enter a sequence into the field and press **Enter**. The fragment found will be highlighted in another color.

Sequence view area

The sequence view area shows chain sequences in one-letter code. You can select residues within this view area. In the **Options** dialog, you can change selection modes and color patterns for the sequence view area, including the background color. Note that selection modes can also be customized on the control panel. A residue marked with a red underscore belongs to an α-helix and that with a blue underscore, to a β-structure.

On the left side of the area you can see chain identifiers selected for viewing. The names of chains containing recently selected residues are highlighted (the highlighting color is set in the **Options** dialog). The background color of chain names is customized in the **Options** dialog . If you click the chain name, the entire sequence will be selected.

The residues you are pointing to with your mouse is highlighted with a user-defined color.

Dialog control buttons

- Click **OK** to apply selections and close the dialog.
- Click **Apply** to apply selections and leave the dialog open.
- Click **Cancel** to close the dialog and cancel the current selections.

Status bar

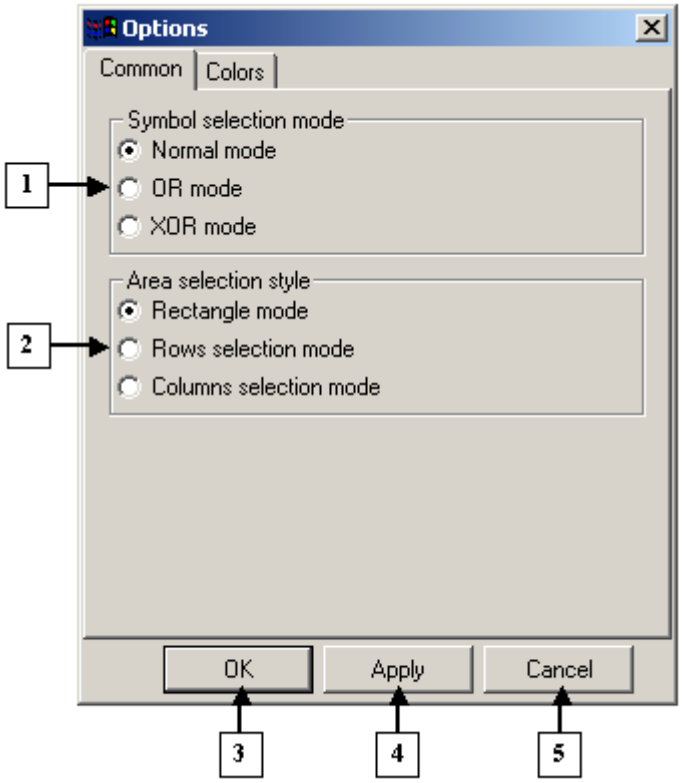
The status bar shows:

- Information about the residue you are pointing to with your mouse: residue name in three-letter code and its number in the PDB file.
- The name of the control panel button you are pointing to with your mouse.

Options of the *Sequence viewer* dialog

To open the **Options** dialog, click the  control panel button in the Sequence viewer dialog. The**Options** has two tabs: the **Common** tab which allows you to adjust selection modes for the **Sequence viewer** dialog and the **Colors** tab which serves to customize the colors of selected residues.

Common tab

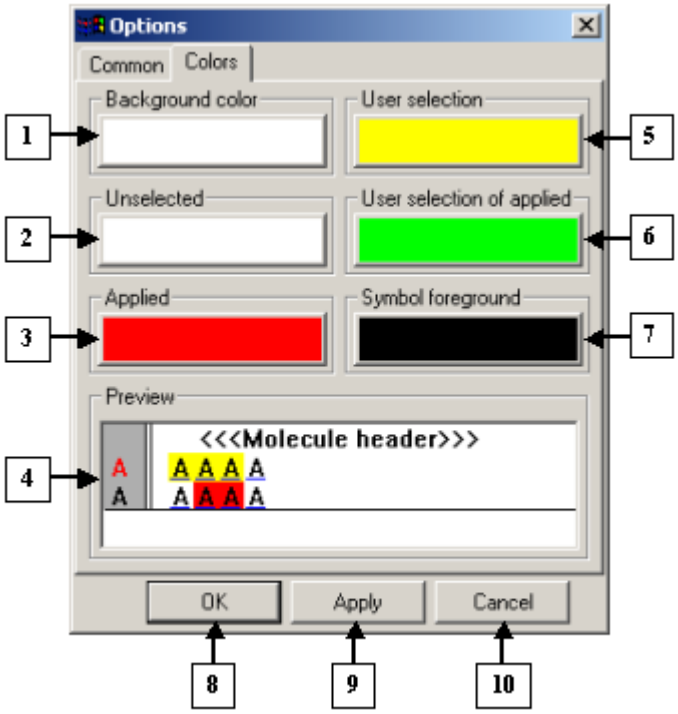


1. The **Symbol selection mode** pane. **2.** The **Area selection style** pane. **3.** The **OK** button. **4.**The **Apply** button. **5.** The **Cancel** button.

- On the **Symbol selection mode** pane, you can set the following selection modes:
  - **Normal mode** - In this mode, each subsequent selection unselects the previously selected item.
  - **OR mode** - In this mode, all subsequent selections are added to the previously selected items.
  - **XOR mode** - In this mode, a previously selected item is unselected by subsequent selection.
- On the **Area selection style** pane, you can change the style of selecting residues in the selection view area:
  - **Rectangle mode** - In this mode, you select a rectangular area while moving your mouse. All residues within this area are automatically selected.
  - **Rows selection mode** - In this mode, you select all residues in a row while moving your mouse.

- **Columns selection mode** - In this mode, you select all residues in a column while moving your mouse.

Colors tab



1. The **Background color** pane. **2.** The **Unselected** pane. **3.** The **Applied** pane. **4.** The**Preview** field. **5.** The **User selection** field. **6.** The **User selection of applied** pane. **7.** The**Symbol foreground** pane. **8.** The **OK** button. **9.** The **Apply** button. **10.** The **Cancel** button.

- On the **Background color** pane, you can select a background color for the sequence view area. The color of the button is the current background color. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.
- On the **Unselected** pane, you can select a color for unselected residues. The color of the button is the current color of unselected elements. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.
- On the **Applied** pane, you can select a color for applied selections. The button displays the current color. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.
- On the **User selection** pane, you can select a color for new selections. The button displays the current color of new selections. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.
- On the **User selection of applied** pane, you can select a color for sections of overlying new and applied selections. The button displays the current color of these sections. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.

- On the **Symbol foreground** pane, you can customize a color of residues. The button displays the current color of symbols. When you click this button, the **Color** dialog appears on your screen. In this dialog, you can select a background color.
- In the **Preview** field, you can preview the customized colors.

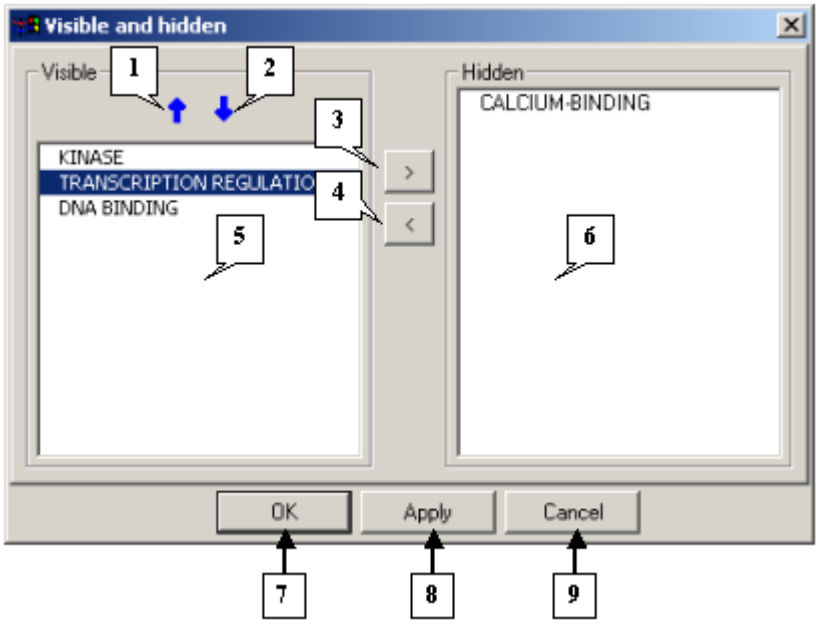
Dialog control buttons

- Click **OK** to apply changes and close the dialog.
- Click **Apply** to apply changes and leave the dialog open.
- Click **Cancel** to close the dialog and cancel changes.

***Visible and hidden elements* dialog**

To open the **Visible and hidden elements** dialog, click the  control panel button in the Sequence viewer dialog. In the **Visible and hidden elements** dialog, you can change the content and order of models and alignments as they are displayed in the sequence view area of the **Sequence viewer** dialog.

The *Visible and hidden* dialog



1. The button for moving the selected models upwards. **2.** The button for moving the selected models downwards. **3.** The button for hiding selected models. **4.** The button for showing selected models. **5.** The **Visible** list. **6.** The **Hidden** list. **7.** The **OK** button. **8.** The **Apply** button. **9.** The**Cancel** button.

To show specific models or alignments, follow these steps:
1. Select the identifiers of models and alignments in the Hidden list by clicking your mouse (if you want to unselect a selected identifier, click it with your mouse).
2. Click the  button. After this, the selected identifiers will be removed from the **Hidden** list and added to the end of the **Visible** list in the same order as they were arranged in the **Hidden** list.

To hide some models, follow these steps:
1. Select the corresponding model identifiers and alignments in the Visible list by clicking your mouse (if you want to unselect a selected identifier, click it with your mouse).
2. Click the  button. After this, the selected identifiers will be removed from the **Visible** list and added to the end of the **Hidden** list in the same order as they were in the **Visible** list.

To change the order of models in the lists, click the  or  buttons to shift a model one step above or below.

Dialog control buttons

- Click **OK** to apply changes and close the dialog.
- Click **Apply** to apply changes and leave the dialog open.
- Click **Cancel** to close the dialog and cancel changes.

Selecting scene elements

You can select specific atoms, chains, residues, and chemical elements to be displayed in a model on the**Model options** dialog. To open this dialog, do the following:

- Select **View>Model** options in the main menu.
- Click the  control panel button.

The information pane displays the following data about all loaded models and for the model selected in the drop-and-down list:
1. The total number of chains, residues, and atoms in models and the number of displayed atoms.
2. The number of selected atoms.

Dialog control buttons

- Click **OK** to apply changes and close the dialog.
- Click **Apply** to apply changes and leave the dialog open.
- Click **Cancel** to close the dialog and cancel changes.

You can select a model in the list of model identifiers and change the parameters of the selected model on the **Atoms**, **Residues**, **Chains**, and **Elements** tabs.

On the **Atoms** tab, you can select atoms to be displayed in the selected model. The list contains the names of atoms in a model. To show or hide atoms, check (☑) or uncheck (☐) the corresponding boxes. Click the control panel buttons to display the following groups of atoms:

All - all atoms in the list.

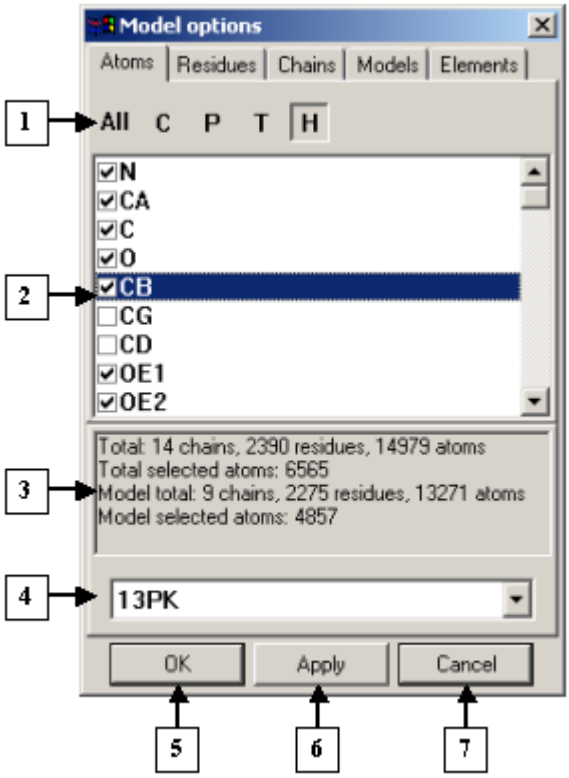
C - protein backbone atoms: Cα, N, C, and O.

P - some of the protein backbone atoms: Cα, N, and C.

T - only Cα- atoms in the protein backbone.

H - all hydrogen atoms are hidden.

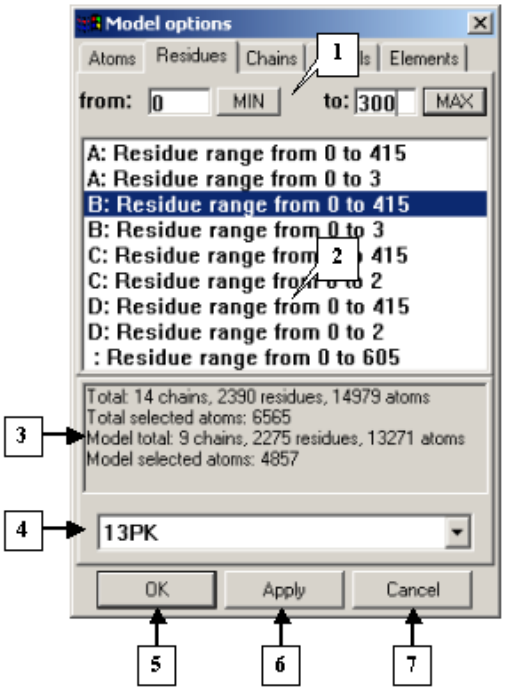
The *Model options* dialog. The *Atoms* tab



1. Control panel. **2.** List of atoms. **3.** Information panel. **4.** List of identifiers of the models loaded.**5.** The **OK** button. **6.** The **Apply** button. **7.** The **Cancel** button.

The **Residues** tab serves to select the residues to be displayed in a model. The list contains chain identifiers with residue ranges for each chain. To change the residue range, select the chain and insert the required values in the **from** and **to** fields. If you click the **MIN** button, the position number of the first residue in the chain appears in the **from** field. If you click the **MAX** button, the position number of the last residue in the chain appears in the **to** field.

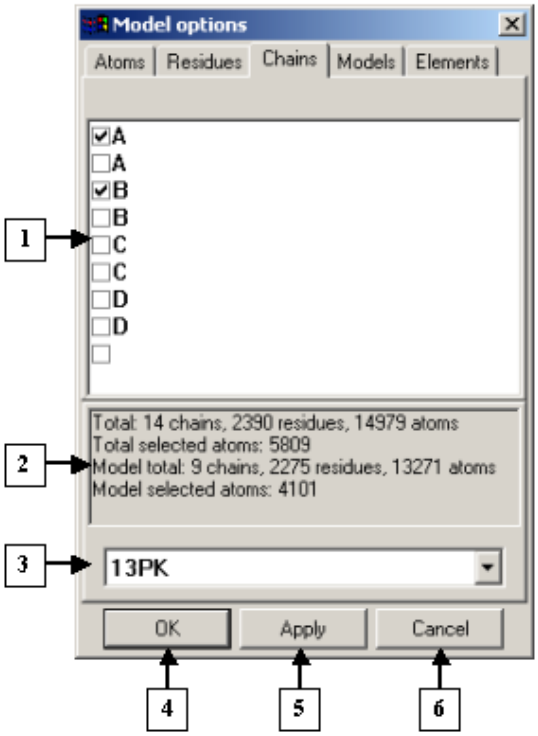
The *Model options* dialog. The *Residues* tab



1. Fields for changing the range of displayed residues. **2.** List of chain identifiers with residue ranges. **3.** Information panel. **4.** Identifiers of the models loaded. **5.** The **OK** button. **6.** The **Apply**button. **7.** The **Cancel** button.

On the **Chains** tab, you can select the chains to be displayed in a model. To show or hide chains, check (☑) or uncheck (☐) the corresponding boxes.

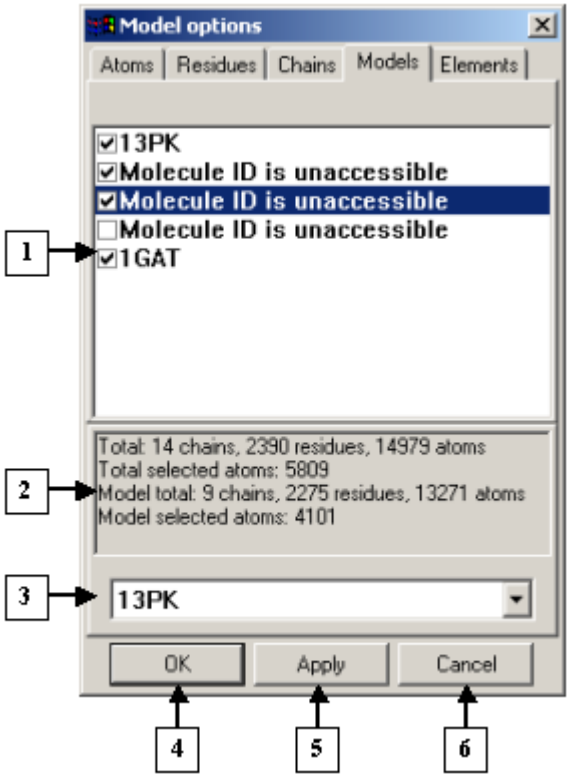
The *Model options* dialog. The *Chains* tab



1. List of chains. **2.** Information panel. **3.** List of identifiers of models loaded. **4.** The **OK** button.**5.** The **Apply** button. **6.** The **Cancel** button.

The **Models** tab serves to select the models to be displayed. The list contains model identifiers. To show or hide models, check (☑) or uncheck (☐) the corresponding boxes.

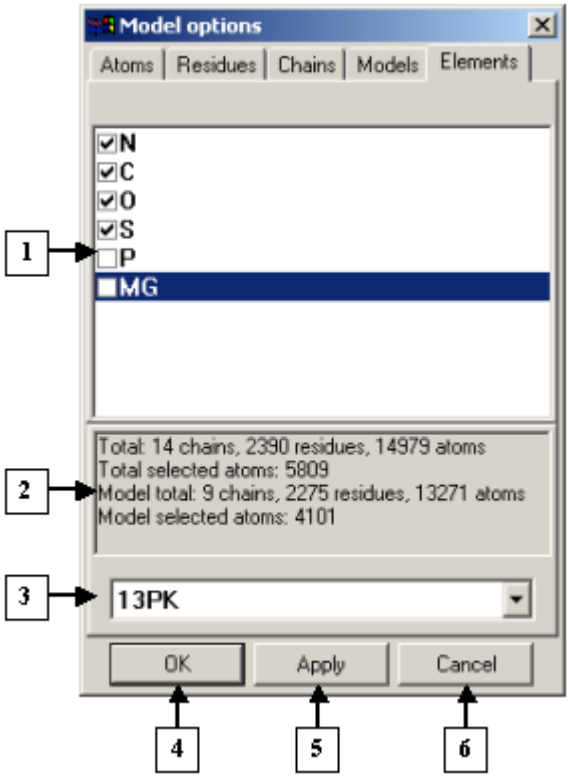
The *Model options* dialog. The *Models* tab



1. Model identifiers list. **2.** Information panel. **3.** List of identifiers of models loaded. **4.** The **OK**button. **5.** The **Apply** button. **6.** The **Cancel** button.

The **Elements** tab serves to select the chemical elements to be displayed in a model. The list contains the names of chemical elements. To show or hide chemical elements, check (☑) or uncheck (☐) the corresponding boxes.

The *Model options* dialog. The *Elements* tab



1. List of chemical elements. **2.** Information panel. **3.** List of identifiers of models loaded. **4.** The**OK** button. **5.** The **Apply** button. **6.** The **Cancel** button.

Options dialog

On the **Options** dialog, you can set the general parameters of the model and mouse parameters. To open the **Options** dialog, do the following:

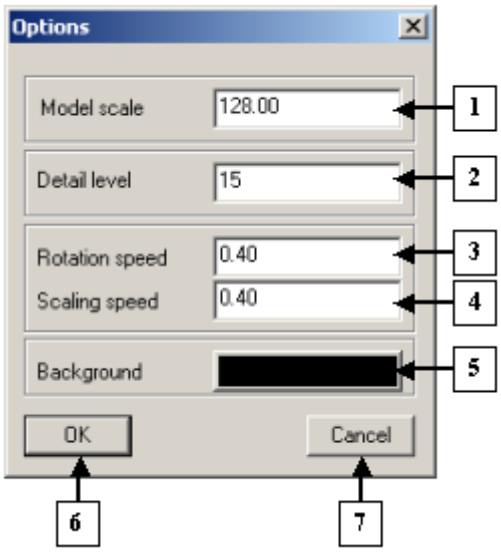
- Select the **View>Options** option in the main menu.
- Click the  control panel button.

In the **Options** dialog, you can change:

- The distance to the model in the **Model scale** field.
- The quality of model images in the **Detail level** field. For example, the value 2 corresponds to the **Very low** detail level (also set by clicking the **View>Detail level>Very low** option in the main menu), 5 to the **Low level**, 15 to the **Normal** level, 25 to the **High** level, and 40 to the**Very high** level.
- The sensitivity of rotation to mouse motion adjusted in the **Rotation speed** field.
- The sensitivity of scaling to mouse motion set in the **Scaling speed** field.

- The background color of the view area. Click **Background** button to open the **Color** dialog and select a background color.

The *Options* dialog.



1. The field for entering the distance to the model. **2.** Detail level. **3.** Rotation speed. **4.** Scaling speed. **5.** The button for selecting the background color for the view area. **6.** The **OK** button. **7.**The **Cancel** button.

Dialog control buttons

- Click **OK** to apply changes and close the dialog.
- Click **Cancel** to cancel changes and close the dialog.

Matrix diagram dialog

In the **Matrix diagram** dialog, you can set the program to display structural features of models as matrix diagrams. To open the **Matrix diagram** dialog, do the following:

- Select the **Window>Matrix viewer** option in the main menu.
- Click the  control panel button.

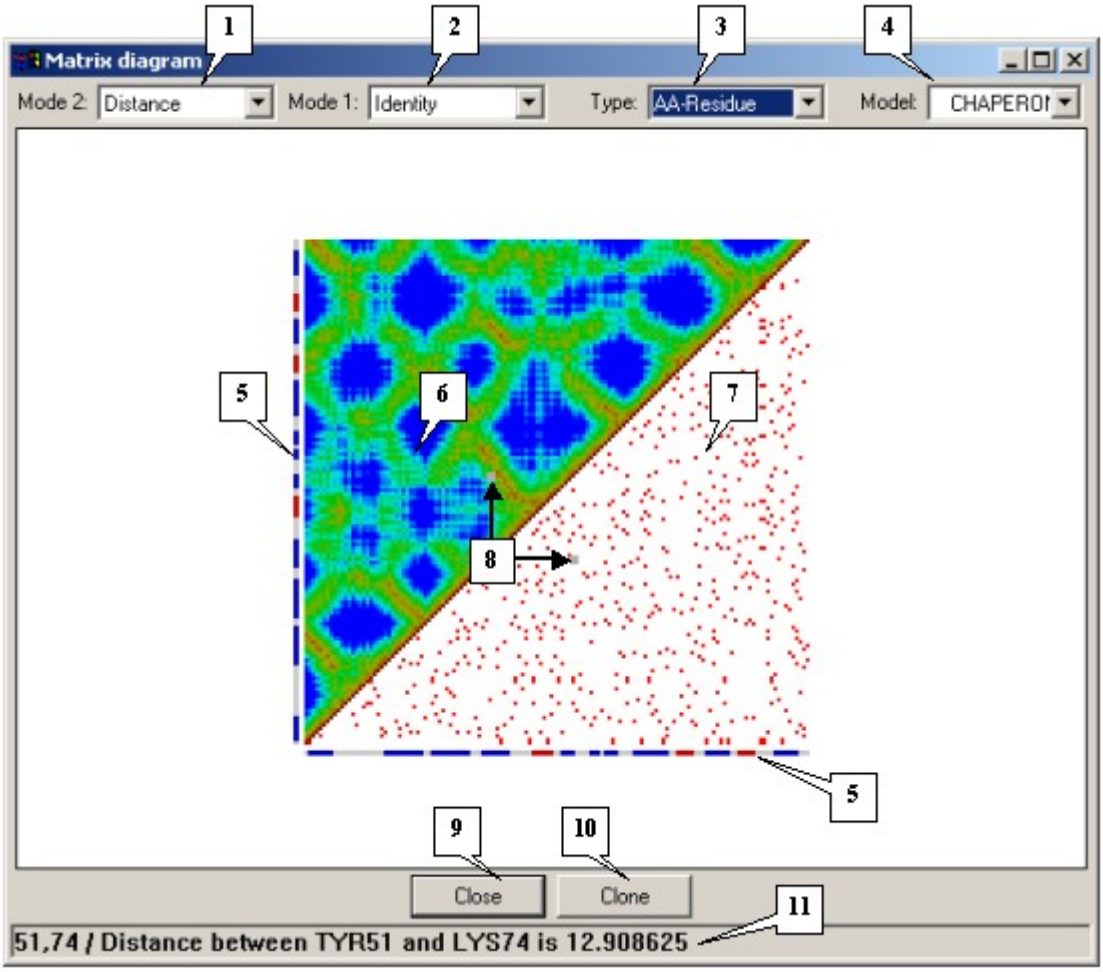
The color of each cell in the diagram depends in the value of the corresponding matrix element. You can change the type and view mode for your matrices.

Use the **Type** drop-and-down list to select the types of elements to be displayed in a matrix diagram. The following variants are available:

- **Residue** - The diagram shows relationships between standard groups of atoms, including aminoacids, nucleotides, and heterogroups.

- **Atom** - The diagram shows relationships between atoms.
- **AA-Residue** - The diagram shows relationships between aminoacid residues.

The *Matrix diagram* dialog.



1. Drop-and-down list for selecting the mode for the upper matrix. **2.** The drop-and-down list for selecting the mode for the lower matrix. **3.** Types of elements. **4.** Model identifiers. **5.** Secondary structure. **6.** Upper matrix. **7.** Lower matrix. **8.** Mouse pointer position. **9.** The **Close** button. **10.**The **Clone** button. **11.** Status bar.

The upper matrix mode can be selected in the **Mode 2** drop-and-down list and the lower matrix mode can be selected in the **Mode 1** drop-and-down list. The following matrix modes are available:

- **Distance** - Show distances between matrix elements.
- **Identity** - Show similarities between the types of elements.
- **SS bond** - Show disulphide bonds.
- **Hydrogen bonds** - Show hydrogen bonds.

In the **Model** drop-and-down list, select the identifier of the model to be displayed as a matrix. The list contains identifiers of all loaded models.

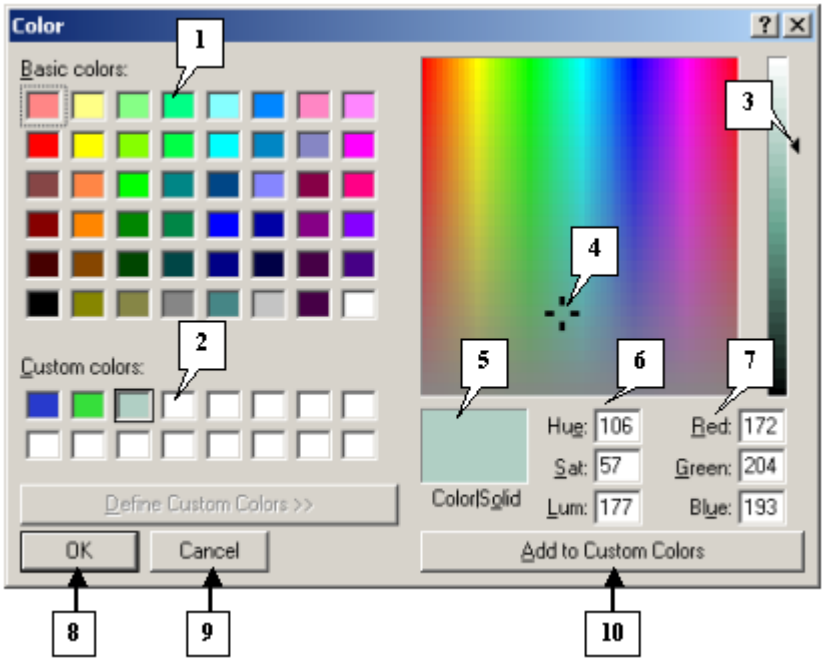
The secondary molecular structure is shown on the left and below the matrix. α-helix fragments are shown in red, β-structures are blue, and turns and non-structured elements are white.

The status bar displays the following data about the pair of elements marked with the mouse pointer in the matrix diagram: the distance between them in the **Distance** mode, their resemblance in the **Identity**mode, the presence or absence of hydrogen bonds in the **Hydrogen bonds** mode, and the presence or absence of disulphide bonds in the **SS bond** mode.

Click the **Clone** button to make a copy of this dialog.

Click the **Close** button to close this dialog.

Color dialog



1. Basic colors. **2.** Custom colors. **3.** Slider. **4.** Color selector. **5.** Current color preview box.**6.** The HSB color model. **7.** The RGB color model. **8.** The **OK** button. **9.** The **Cancel** button.**10.** The **Add to Custom Colors** button.

In the **Color** dialog, you can select colors of your models.

To change colors, do one of the following:

- **Basic colors**. Click a color box to change the basic color. You will see the new color in the color preview box. To confirm your selection, click **OK**.
- **Custom colors**. Click the color selector and pick the required color. You will see the new color in the color preview box. To confirm your selection, click **OK**.

- **New color**. To add a new color, you can move a slider, color selector, or the HSB or RGB color fields. The new color will appear in the color preview box. To confirm your selection, click **OK**.

Note. To change a custom color, click the custom color box and then change the color by moving the slider selector or inserting the required values in the HSB or RGB color fields. After this, click the **Add to Custom Colors** button. The new custom color will appear in the custom color boxes.

Dialog control buttons.
Click the **OK** button to apply changes and close the dialog.
Click the **Cancel** button to cancel changes.

References

1. http://www.wwpdb.org/docs.html
2. Shindyalov IN, Bourne PE (1998) Protein structure alignment by incremental combinatorial extension (CE) of the optimal path. Protein Engineering 11(9) 739-747.

3. www.softberry.com/berry.phtml?topic=getatoms&group=help&subgroup=propt