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1. 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. Models (or selected parts of models) can be moved, rotated and zoomed in or out.

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.

1.1. Installation procedure for MS WINDOWS Tm

For installation of 3D-Explorer Trial version, the following steps are required:

1. Download the archive;
2. Extract files from archive with full pathways

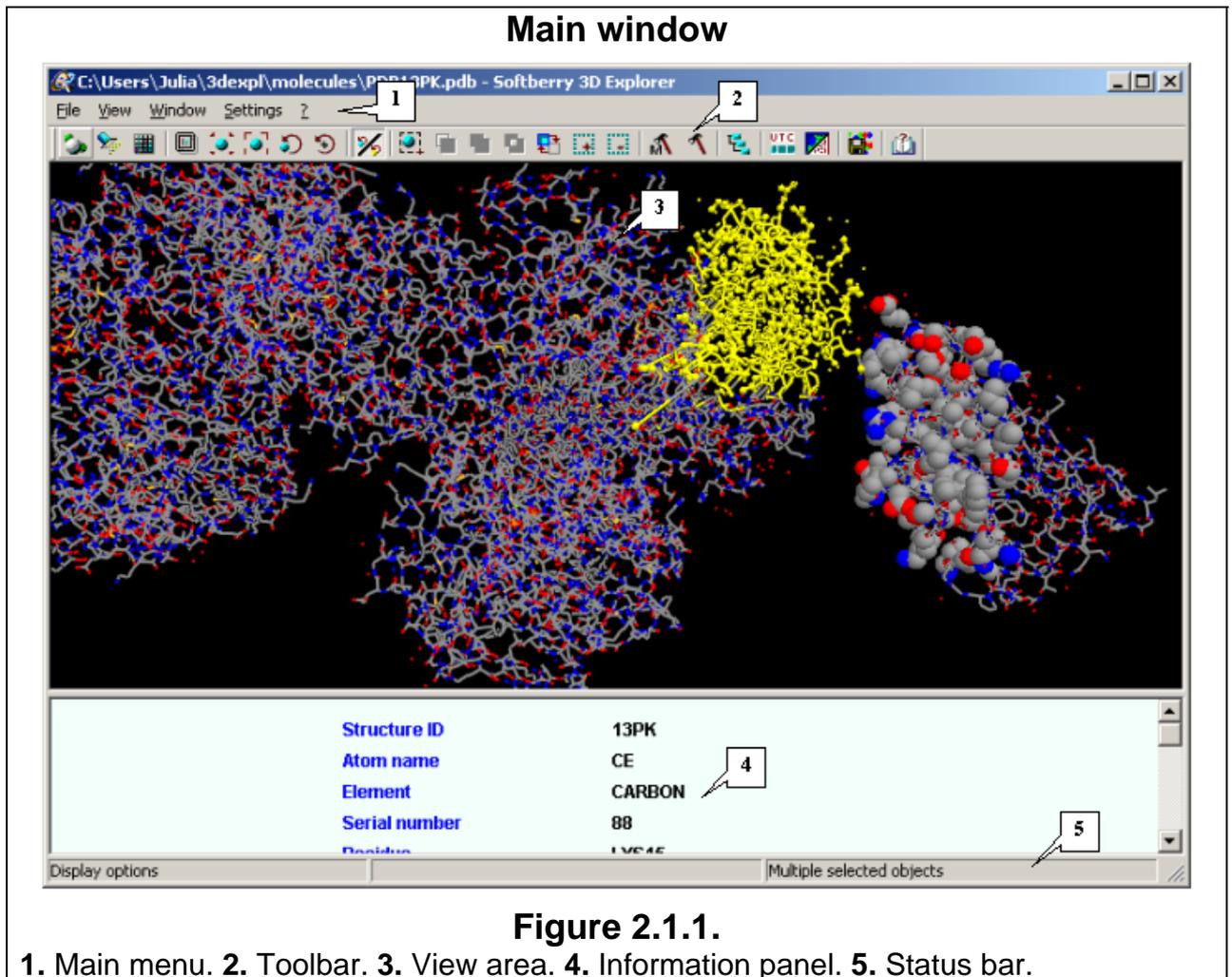
To run the application use 3DExplorer.exe file in the "rbin" folder.

2. General description of the program

2.1. Main window

The 3D-Explorer main window consists of the following elements (Fig. 2.1.1):

- Main menu
- Toolbar
- View area
- Information panel
- Status bar



2.2. Main menu commands

The **File** menu contains the following commands:

- **Open** – Load a model.
- **Add** – Add a model to the scene.
- **Load from PDB** – opens “Load from PDB” dialog window, purposed for loading of a PDB-file from PDB-server.
- **Open NMR** – opens “Open NMR” dialog window, purposed for loading of a file with structures, obtained with use of Nuclear Magnetic Resonance.
- **Align 2 3D** – opens “Select chains” dialog window, purposed for defining the parameters of loaded alignment.
- **Getatoms** – opens “Getatoms” dialog window, purposed for loading of «GetAtoms» program work results.
- **Exit** – Quit the program.

The **View** menu contains the set of commands, purposed for working with model's image:

- **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 window where you can set the delay for model rotation.
- **Display** – Open the **Display options** dialog window to customize the geometry and color settings for the model.
- **Light options** – Open the **Light options** dialog window to customize settings for lighting the model.
- **Colors** – Open the **Color dialog window** to select colors for particular chemical elements.
- **Model options** – Open the **Model Options** dialog window to select the types of atoms, chains, aminoacid residues, and chemical elements to be displayed in the model.
- **Options** – Open the **Options** dialog window to customize the general view of the model and mouse settings.
- **Fullscreen** – Display the view area in full-screen mode.
- **Save scene to Bitmap** – opens “Save as” dialog window, purposed for saving of the scene image as a graphic file. In order to save an image, define the name and graphic format of a file and then press “Save” button. Available formats are: bmp, jpeg, gif, png, tiff.

The **Window** menu contains the following commands:

- **Tree dialog** – Display the **Tree explorer** dialog window to view the hierarchical structure of the molecular elements.
- **Sequence viewer** – Open the **Sequence viewer** dialog window to display sequences of protein chains.
- **Matrix dialog** – Open the **Matrix diagram** dialog window to display specific features of the molecular structure as a matrix diagram.
- **View PDB file** – opens “PDB data” dialog window (fig. 2.2.1), purposed for viewing and saving of PDB-file.

The *PDB data* dialog window

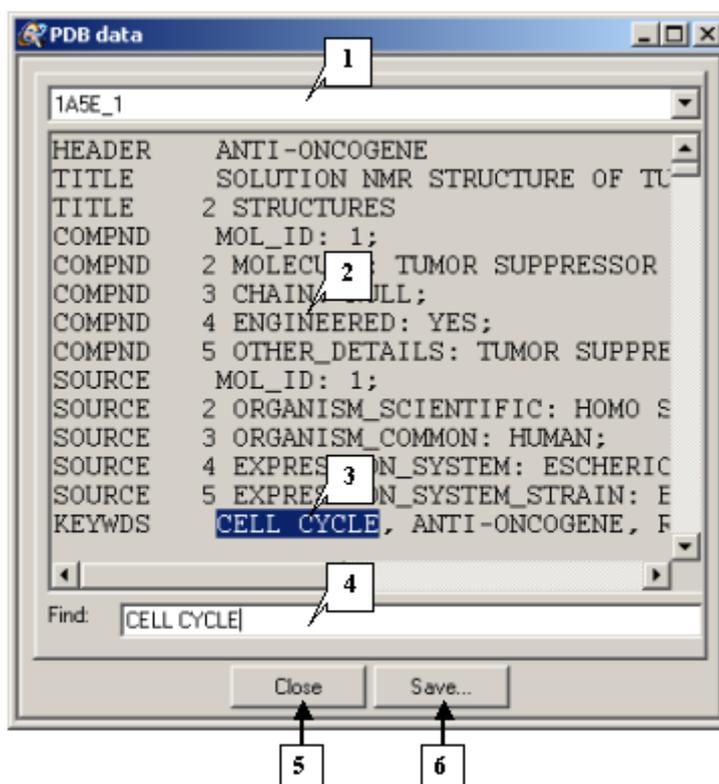


Figure 2.2.1.

1. The list of loaded structures.
2. PDB-file for selected in the list structure.
3. Found substring.
4. Entry field for substring to search.
5. Button for closing of the window.
6. Button for saving of the PDB-file.

The **Settings** menu has a set of commands for configuring application settings:

- **Network settings** – Open the **Network settings** dialog window (Fig. 2.2.2) to configure network settings.

The *Network settings* dialog window

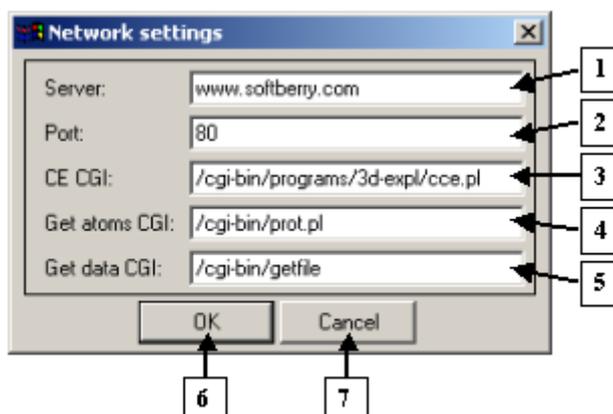


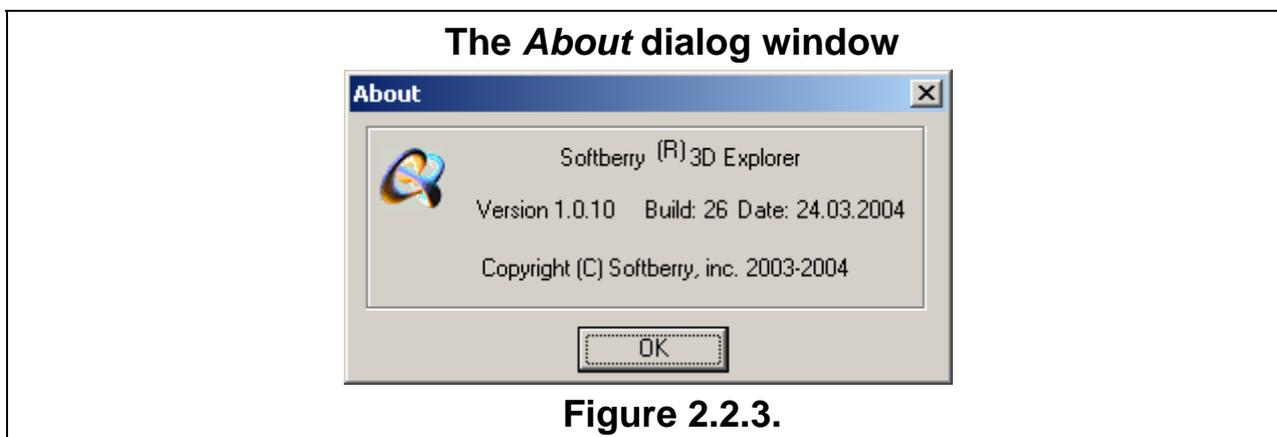
Figure 2.2.2.

1. Server address field.
2. Server port field.
3. CE program name field.
4. Getatoms program name field.
5. Get data program name field.
6. Click OK to apply changes and

close the dialog window. **7.** Click Cancel to cancel changes and close the dialog window.

The ? menu has the commands:

- **Help** – Refer to Help Topics.
- **About** – Open the **About** dialog window with information about the program (Fig. 2.2.3).



2.3. Toolbar

The 3D-Explorer toolbar has the following buttons (Click the button ... to...):

	Display options - Open the Display options dialog window to customize the geometry and color settings for the model. This button corresponds to the View>Display style menu command.
	Light options – Open the Light options dialog window to customize settings for lighting the model. This button corresponds to the View>Light options menu command.
	Color options –Open the Color dialog window to select colors for specific chemical elements. This button corresponds to the View>Colors menu command.
	Full screen – Display the view area in full-screen mode. This button corresponds to the View>Fullscreen menu command.
	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 window to select the types of atoms, chains, aminoacid residues, and chemical elements to be displayed by the program. This button corresponds to the View>Model options menu command.
	Options – Open the Options dialog window to customize the general view of the model and mouse settings. This button corresponds to the View>Options menu command.
	Tree model dialog – Open the Tree dialog window to view the hierarchical structure of the model elements. This button corresponds to the Window>Tree dialog menu command.
	Sequence viewer – Open the Sequence viewer dialog window to display sequences of protein chains. This button corresponds to the Window>Sequence menu command.
	Matrix viewer – Open the Matrix diagram dialog window to display specific features of the molecular structure as a matrix diagram. This button corresponds to the Window>Matrix dialog menu command.
	Save scene as image – To save the image of scene. It opens the “Save as” dialog window, purposed for saving of the scene’s image as a graphics file.
	Help – Refer to Help Topics. This button corresponds to the ?>Help menu command.

Comment. Place your mouse pointer over a toolbar button to see the function of this button in the status bar (Fig. 2.1.1).

2.4. View area

The view area displays models in the user-defined view mode (Fig. 2.1.1). 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 window to change the background color of the view area (see Section 3.7).

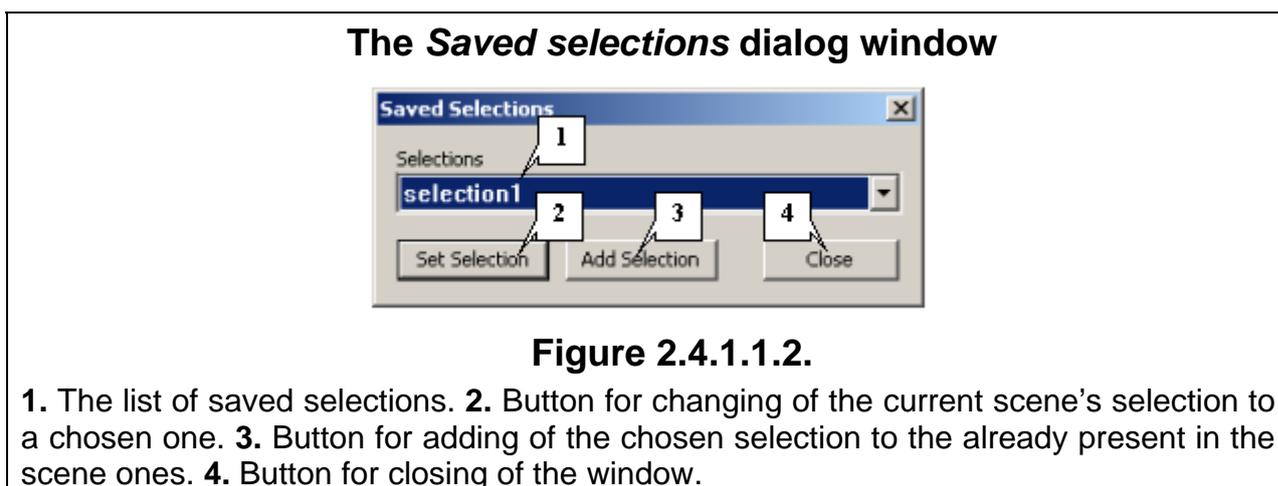
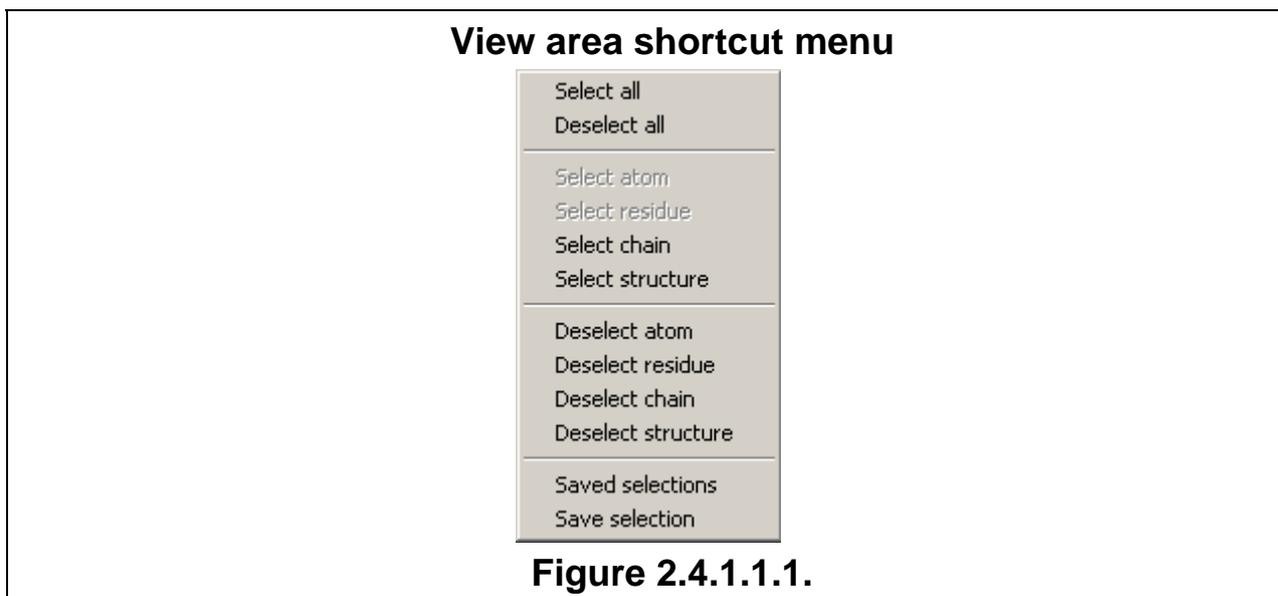
You can move the border between the view area and the information panel by dragging it with your mouse.

2.4.1.1. Shortcut menu

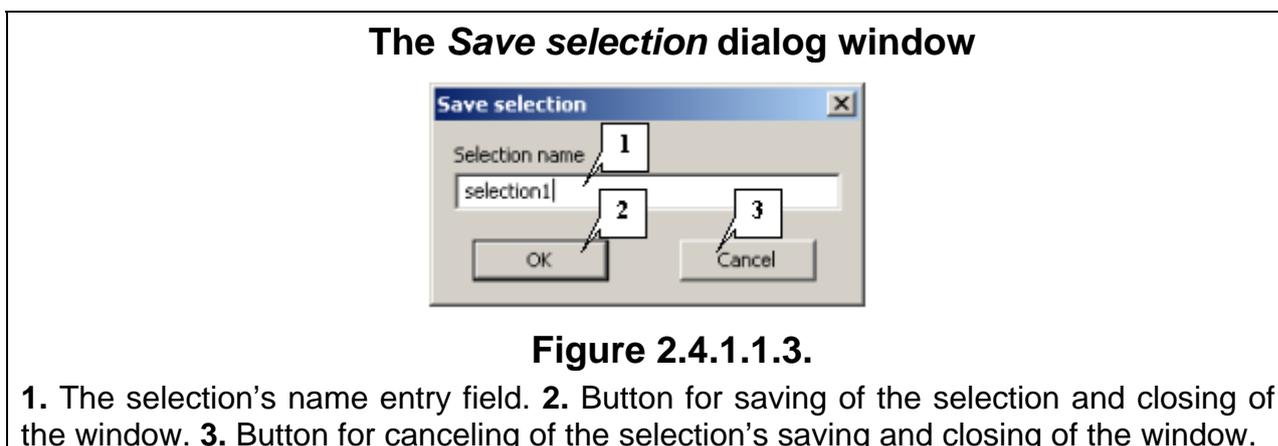
To open a shortcut menu (Fig. 2.4.1.1.1), right-click the view area. The shortcut menu includes the following items:

- **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.
- **Deselect structure** – Deselect a model.
- **Saved selections** – opens the “Saved selections” dialog window, purposed for choosing of saved selections (fig. 2.4.1.1.2). 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.



- **Save selection** – opens the “Save selection” dialog window, purposed for saving of the current selection (fig. 2.4.1.1.3.). It requires to enter the name of selection and press the “OK” button.



2.5. Information panel

The information panel (Fig. 2.1.1) 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.
- PDB-identifier of a structure, at which cursor is pointed, or file's name, from which a structure is loaded (in the case of PDB- identifier's missing).

2.6. Status bar

The status bar (Fig. 2.1.1) displays:

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

3. Working with the system

3.1. Loading a model

3D-Explorer allows the user to load the following models:

- PDB files.
- Files created and edited with the GetAtoms program.
- Alignments created with the CE program.

When a model is being loaded, you can see an information box that disappears after the load is completed (Fig. 3.1.1).

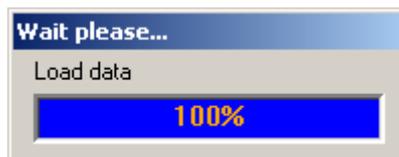


Figure 3.1.1.

- **Load from PDB** - opens the **Load from PDB** dialog window, purposed for loading of a PDB-file from the PDB server.
- **Open NMR** - opens the **Open NMR** dialog window, purposed for loading of a file with structures, obtained with use on nuclear magnetic resonance.
- **Align 2 3D** – opens the **Select chains** dialog window, purposed for defining of the loading alignment's parameters.
- **Getatoms** – opens the **Getatoms** dialog window, purposed for loading of GetAtoms program's working results.

3.1.1. Loading a file

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

3.1.2. Adding a model

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

3.1.3. Loading of PDB-file

The **Load from PDB** dialog window (fig. 3.1.3.1), purposed for loading of a PDB-file from the official PDB server (www.pdb.org), can be opened using the **File> Load from PDB** command of the main menu.

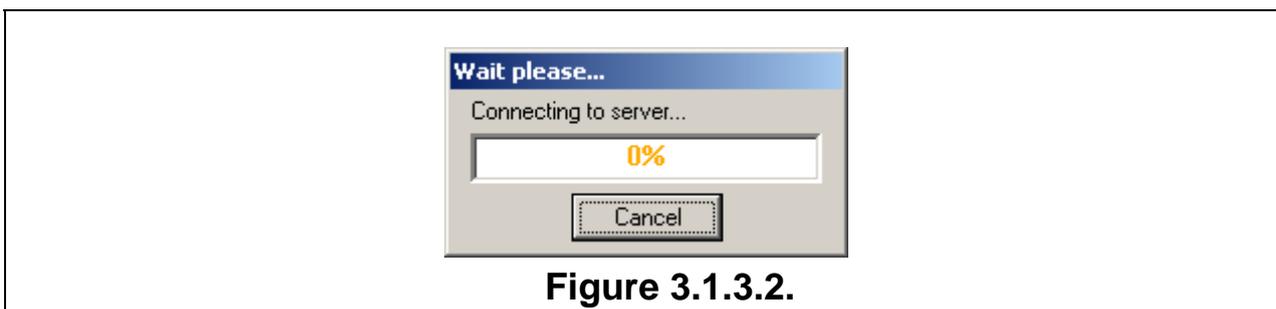
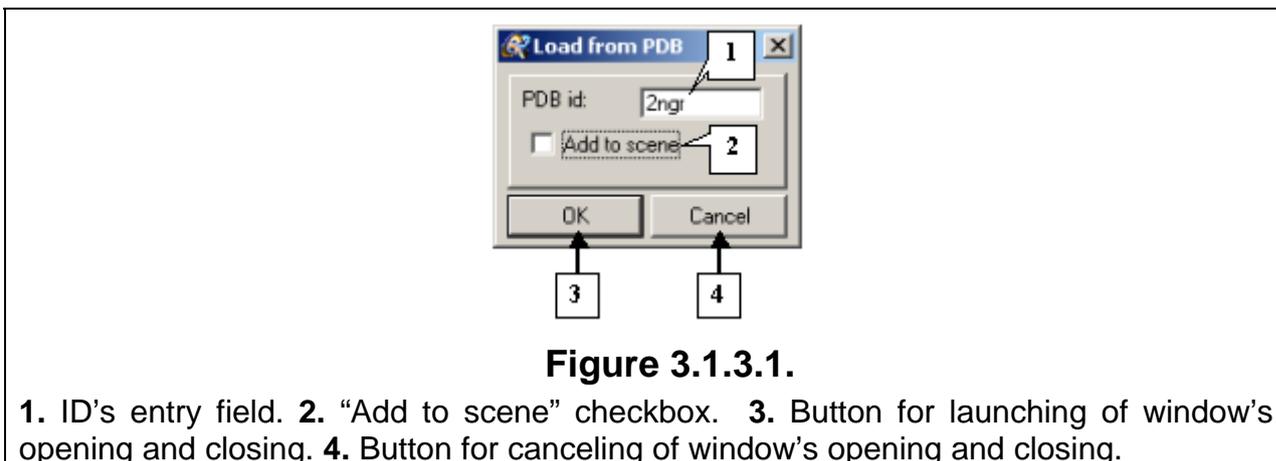
The **PDB id** field is used for specification of the PDB-identifier.

Checkbox **Add to scene**. If the checkbox is checked in, the model is added to scene. If checkbox is checked out, the model substituted the scene's content.

The **OK** button is used for closing of the window and starting of file's loading. During the file's loading appears the information window, which disappears on loading is finished (fig. 3.1.3.2).

The **Cancel** button is used for closing of the window and canceling of file's loading.

The *Load from PDB* dialog window



3.1.4. Loading of NMR-file

The **Open NMR** dialog window (fig. 3.1.4.1), purposed for loading of a file with structures, obtained with use on nuclear magnetic resonance, can be opened using the **File>Open NMR** command of the main menu.

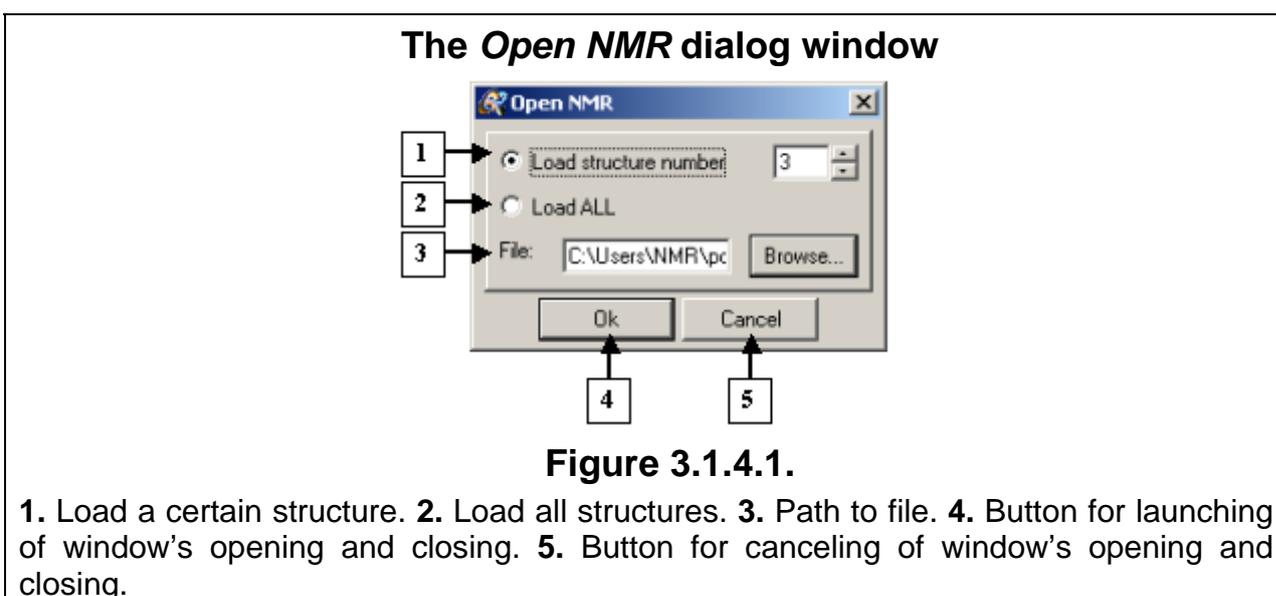
The **Load structure number** option is used for loading of a selected structure.

The **Load all** option is used for loading of all structures from the file.

The **File** field is used for file's full name prompting.

The **OK** button is used for launching of window's opening and closing.

The **Cancel** button is used for canceling of window's opening and closing.



3.1.6. Loading GetAtoms files

Click **File>Getatoms** in the main menu to open the **Getatoms** dialog window (Fig. 3.1.6.1). In this dialog window, you can calculate the coordinates of side chains of amino-acid residues using the coordinates of the atoms in the main chain of the template structure performed by the GetAtoms program and load the model obtained.

Getatoms dialog window interface:

The **Getatoms** dialog window consists of three panes where you can enter the following data:

- Coordinates of the atoms in a template chain.
- Pair alignment of sequences of the calculated and template chains.
- Calculation parameters.

To specify the coordinates of the atoms in a template chain, do one of the following:

- In the **Enter PDB identifier** field, enter the PDB identifier of the template chain from the PDB database. In this case, the coordinates in PDB format will be loaded from the server.
- In the **Or file in PDB format** field, select the PDB file with the user data using the **Browse...** button.

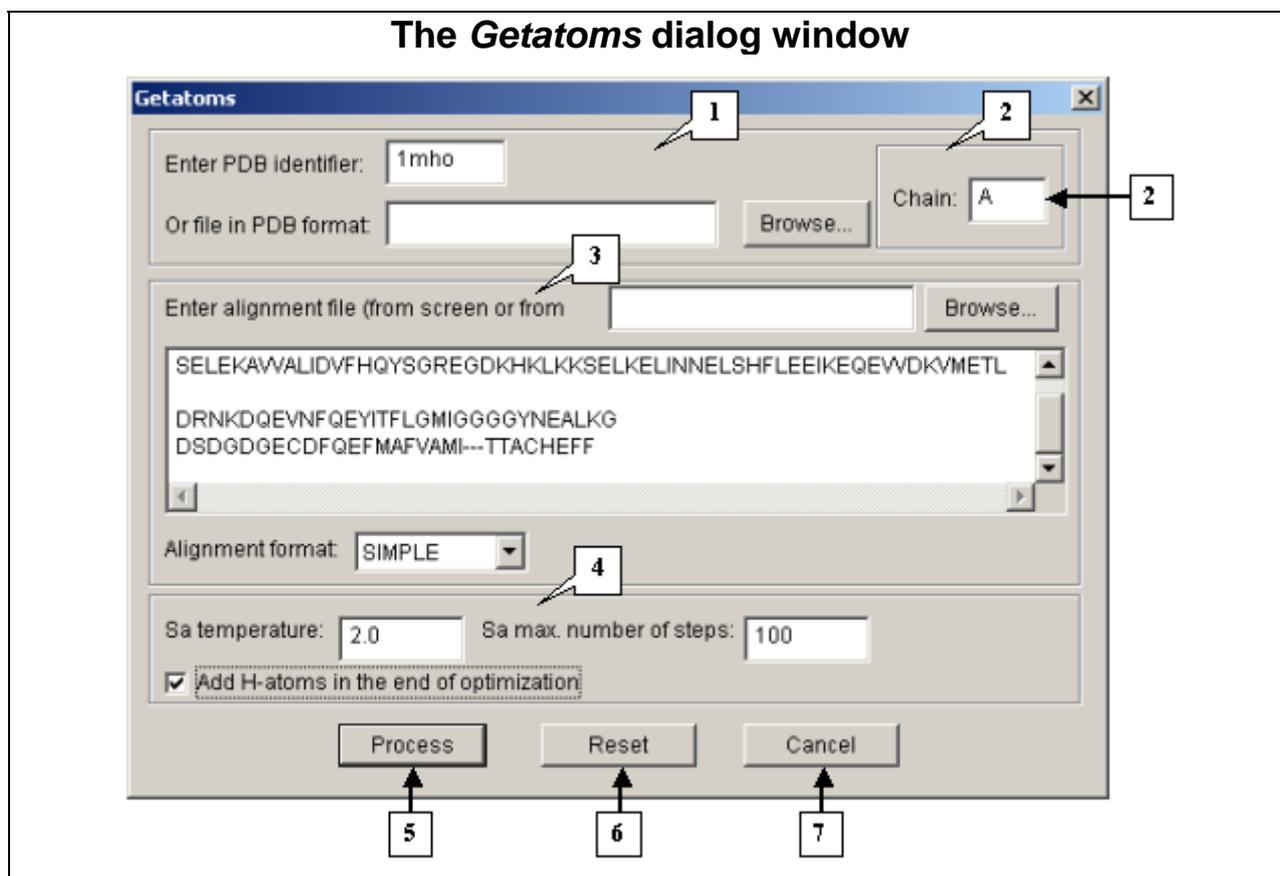


Figure 3.1.3.1.

1. Entry panel for PDB-file of the template strand. 2. Entry field for strand's ID. 3. Panel for defining the parameters of alignment. 4. Panel for defining the parameters of calculations. 5. Button for starting calculations and following loading. 6. Button for clearing "Enter PDB identifier", "Or file in PDB format", "Chain" and "Enter alignment file" fields. 7. Button for canceling calculations.

The **Chain** field serves to specify the identifier of the chain of a template structure.

To specify the alignment for sequences of the calculated and template structures, do one of the following:

- Specify a file with the alignment.
- Insert alignment into the text field.

The **Alignment format** drop-and-down list contains four values [2, 3]:

- LOCAL – Output alignment format of the FOLD program.
- CE – Output alignment format of the CE alignment application.
- FASTA – FASTA format
- SIMPLE – simple format.

To set the calculation parameters, do the following:

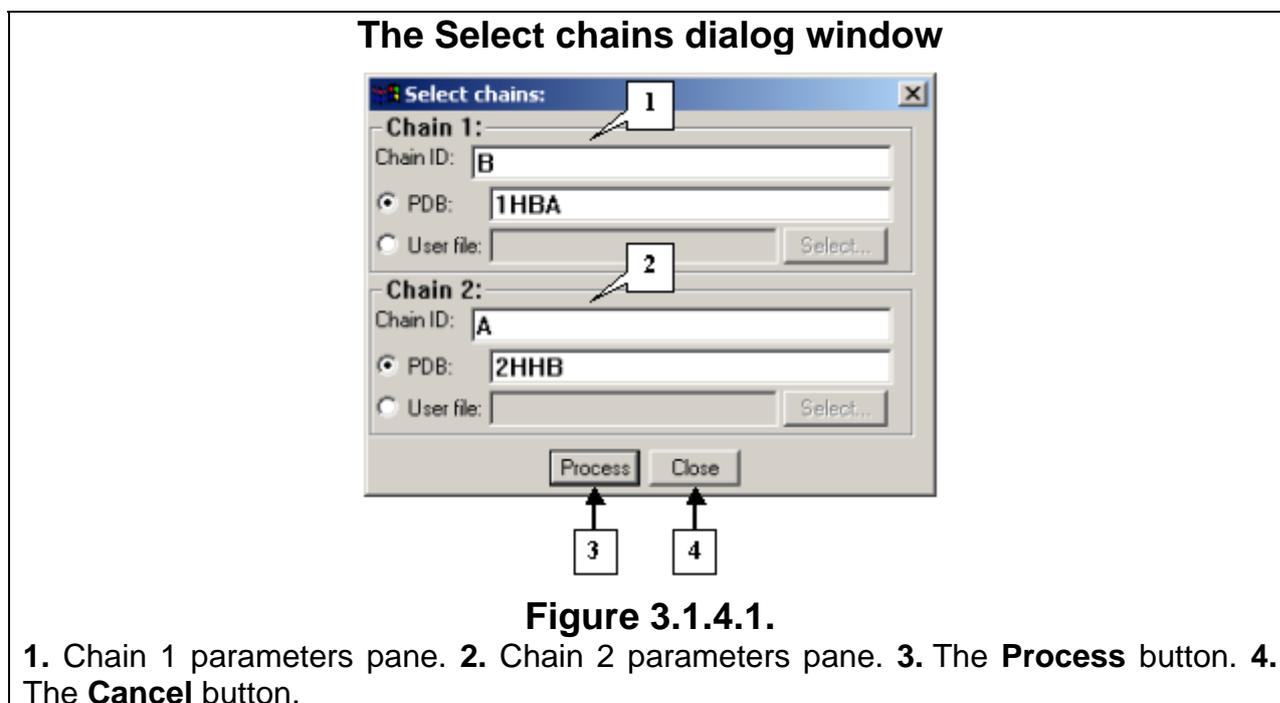
- In the **Sa temperature** field, enter the value of the annealing temperature. The value must be nonzero.
- In the **Sa max. number of steps** field, enter the maximum number of annealing steps.
- Check the **Add H-atoms in the end of optimization** box to add hydrogen atoms. The hydrogen atoms are added according to geometry rules; their position cannot be optimized.

Control buttons

- Click **Process** to start calculating and load the model.
- Click **Reset** to clearing “Enter PDB identifier”, “Or file in PDB format”, “Chain” and “Enter alignment file” fields.
- Click **Cancel** to cancel the calculation.

3.1.4. Loading the alignments created in the CE program.

The **Select chains** dialog window (Fig. 3.1.3.2) allows you to work with the results of the CE program. To open this dialog window, click **File>Align 2 3D** in the main menu.



In the **Chain 1** and **Chain 2** panes, you can specify the following chain parameters.

Use the **Chain ID** field to specify the chain identifier. To define the chain identifier, do one of the following:

- Enter the PDB identifier from the PDB database into the **PDB** field. In this case, the PDB file will be loaded from the server.
- Check the **User file** option button and select a PDB file with the user data

Dialog window control buttons

- Click **Process** to start calculating and load the model.
- Click **Cancel** to cancel the calculation.

3.2. Operations with image.

3.2.1. Setting up the image

3.2.1.2. Setting up the model's view

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

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

The **Display options** dialog window 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 (Fig. 3.2.1.2.1) 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.
- Molecule surface – the surface of the protein molecule (atoms of a solvent and heteroatoms are not considered on building the surface);

List **Styles** for **Molecule surface** group contains the following options:

- **Vertex surface** – the surface is displayed as dots;
- **Wire surface** – the surface is displayed as grid.
- **Solid surface** – «continuous» surface.

Radius of a solvent is defined in **Solvent radius** field, factor of smoothing – in **Smooth factor** field, quality of a surface – in **Voxel count** field at **Surface** panel of **Sizes** tab.

Comment. To build a surface the adopted algorithm «marching cubes» [4] is used.

The viewing parameters for a group can be adjusted by selecting the required values in the following columns:

- The **Modes** checkboxes are used to display/hide certain groups in a model. For the **Protein backbone** group, select an appropriate value from the drop-and-down list to specify protein backbone atoms to be displayed in the model.
- In the **Styles** column, select a style for displaying a group;
- In the **Schemes** column, select a color mode for the elements of a group. Use the **Custom** option to choose other colors.

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: C α , N, C, and O.
- **Partial** – Display only some protein backbone atoms: C α , N, and C.
- **Trace** – Display only C α 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 Heterogeneous 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** panel 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** panel 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** panel of the **Sizes** tab.

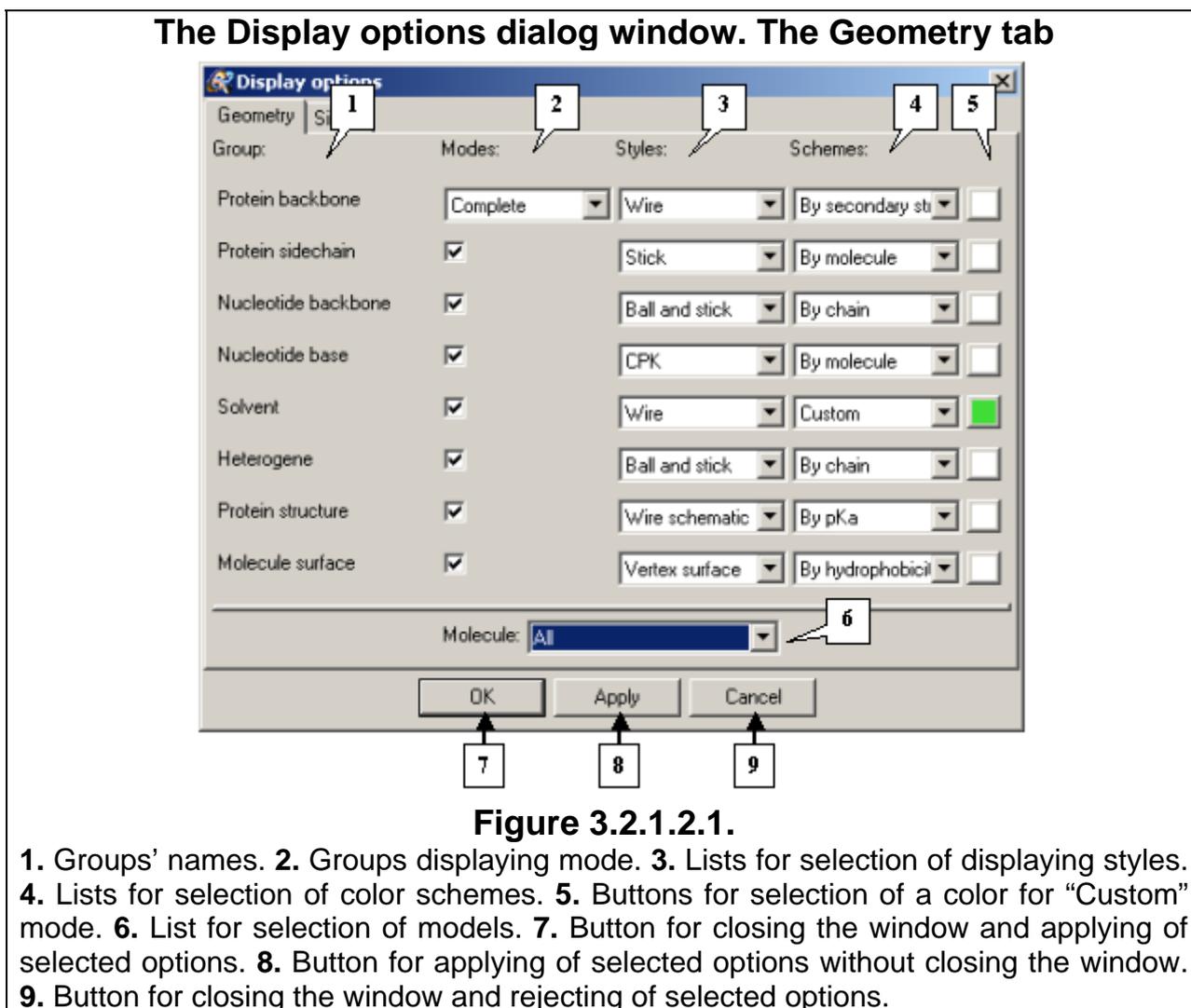
The **Styles** list for the **Protein structure** group contains the following options:

- **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** panel 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 -helices 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 -helices, in the **Helix radius** field on the **Schematic** panel of the **Sizes** tab.
- **Wire trace** – Display traces connecting the $C\alpha$ atoms of the backbone.
- **Solid trace** – Show sticks connecting the $C\alpha$ -atoms of the backbone. The stick radius is set in the **Trace radius** field on the **Trace** panel 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** panel 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 window**, see Section 3.2.3).
- **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 the surface dot is defined by the density of hydration energy (hydrophobic properties of the neighbor atoms in protein molecule)
- **By atom hydrophobicity** – the color of the group's element is defined by hydrophobic properties of the atom.
- **By residue hydrophobicity** – the color of the group's element is defined by hydrophobic properties of the residue, which it belongs to.
- **By charge** – the color of the surface dot is defined by the electrostatic potential of protein molecule.

- **By atom charge** – the color of the group's element is defined by the atom's charge.
- **By pKa** – the color of the group's element is defined by the value of pKa constant.
- **By Secondary structure** – the color of elements in a group depends on the secondary structure of a chain fragment. α -helices 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 window (see Section 3.9) where you can select a color.



Comment.

For **Protein backbone** and **Protein sidechain** groups, list **Schemes** contains all above-mentioned modes excepting **By hydrophobicity** and **By charge** ones.

For **Nucleotide backbone**, **Nucleotide base**, **Solvent** and **Heterogene** groups, list **Schemes** contains **By Element**, **By Residue**, **By Chain**, **By molecule** and **Custom** modes only.

For **Protein structure** group, list **Schemes** contains all modes excepting **By Element**, **By hydrophobicity** and **By charge** ones.

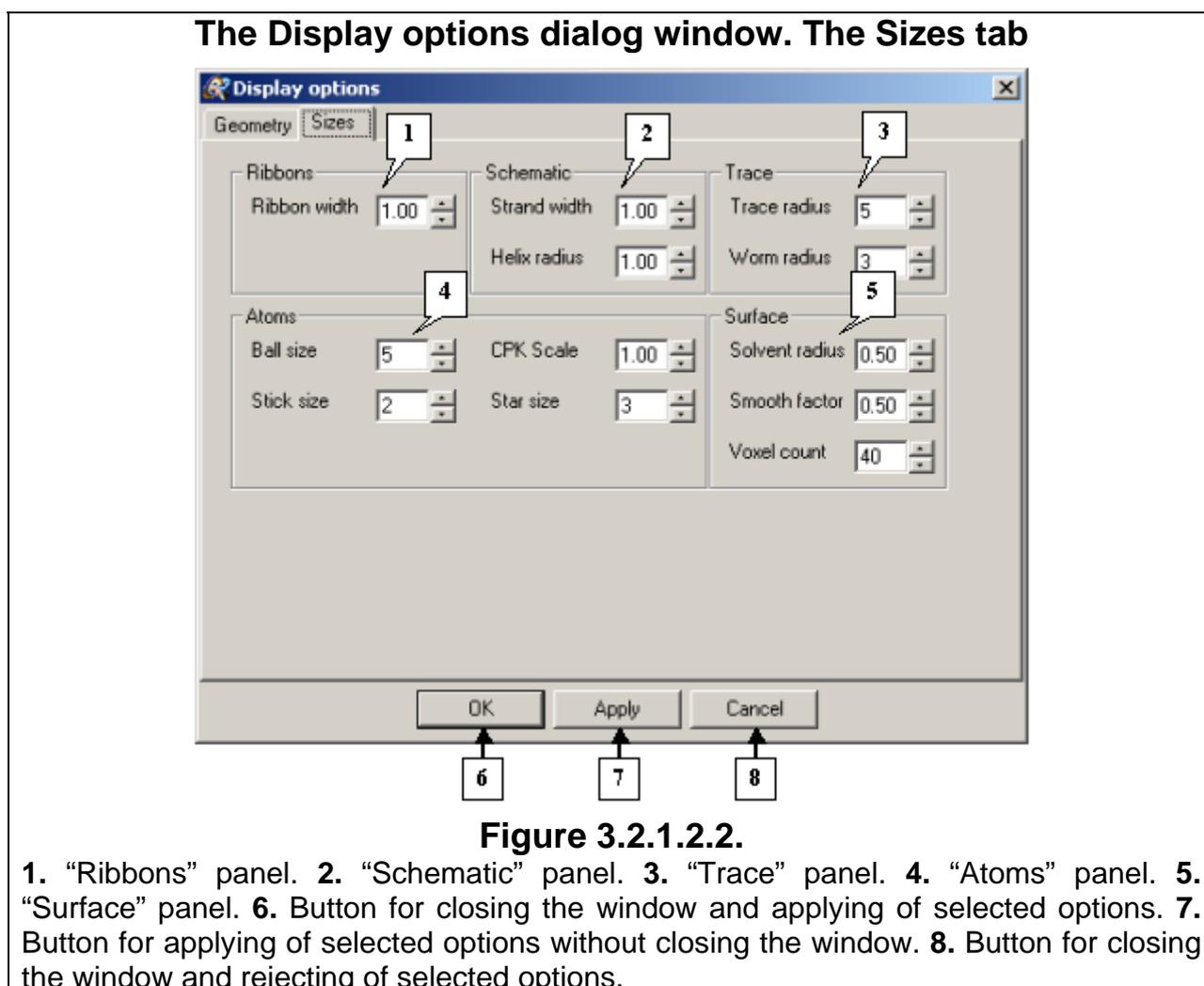
For **Molecule surface** group, list “Schemes” contains the following modes: **By hydrophobicity**, **By charge** and **Custom**.

List **Molecule** is purposed for selecting the models that will be affected by changes, made on **Geometry** tab.

Sizes tab

On the **Sizes** tab (Fig. 3.2.1.2.2) you can change the geometrical parameters of models.

- The **Ribbons** panel 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** panel 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 -helices.
- The **Trace** panel 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** panel 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).
- Panel **Surface** is purposed for changing the parameters of surfaces displaying:
 - Field **Solvent radius** is purposed for changing the radius of solvent.
 - Field **Smooth factor** is purposed for changing the value of smoothing factor. This parameter regulates the preciseness of molecule's contour replication. The less parameter's value, the better surface fits a molecule, however, at small values some defects in surface may appear.
 - Field **Voxel count** is purposed for regulating the quality of surface. The greater parameter's value, the better quality, however, on increasing this value, the time consumption for calculations is also increased.

3.2.2. Light options

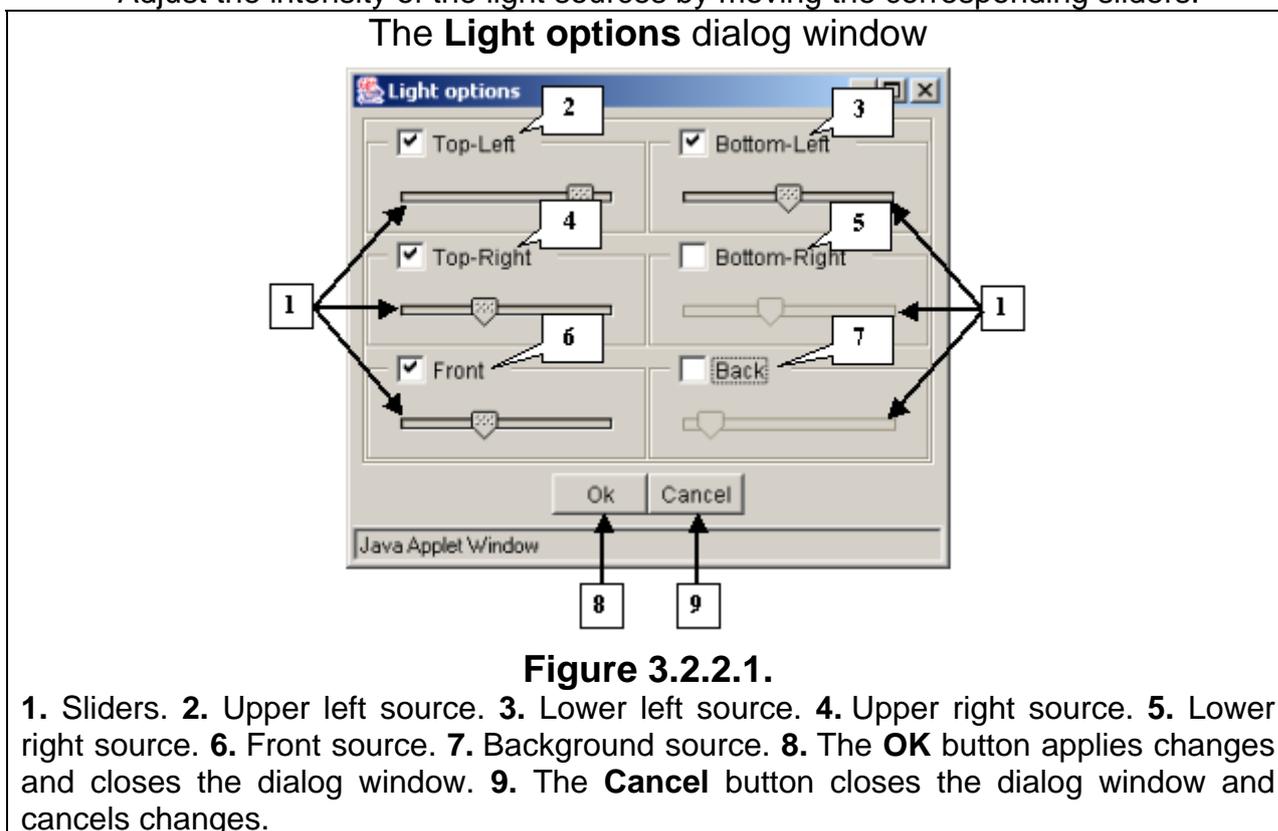
To open the **Light options** dialog window (Fig. 3.2.2.1), do one of the following:

- 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.



3.2.3. Selecting colors of chemical elements

You can change the colors of chemical elements in the **Color dialog window** (Fig. 3.2.3.1). To open this dialog window:

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

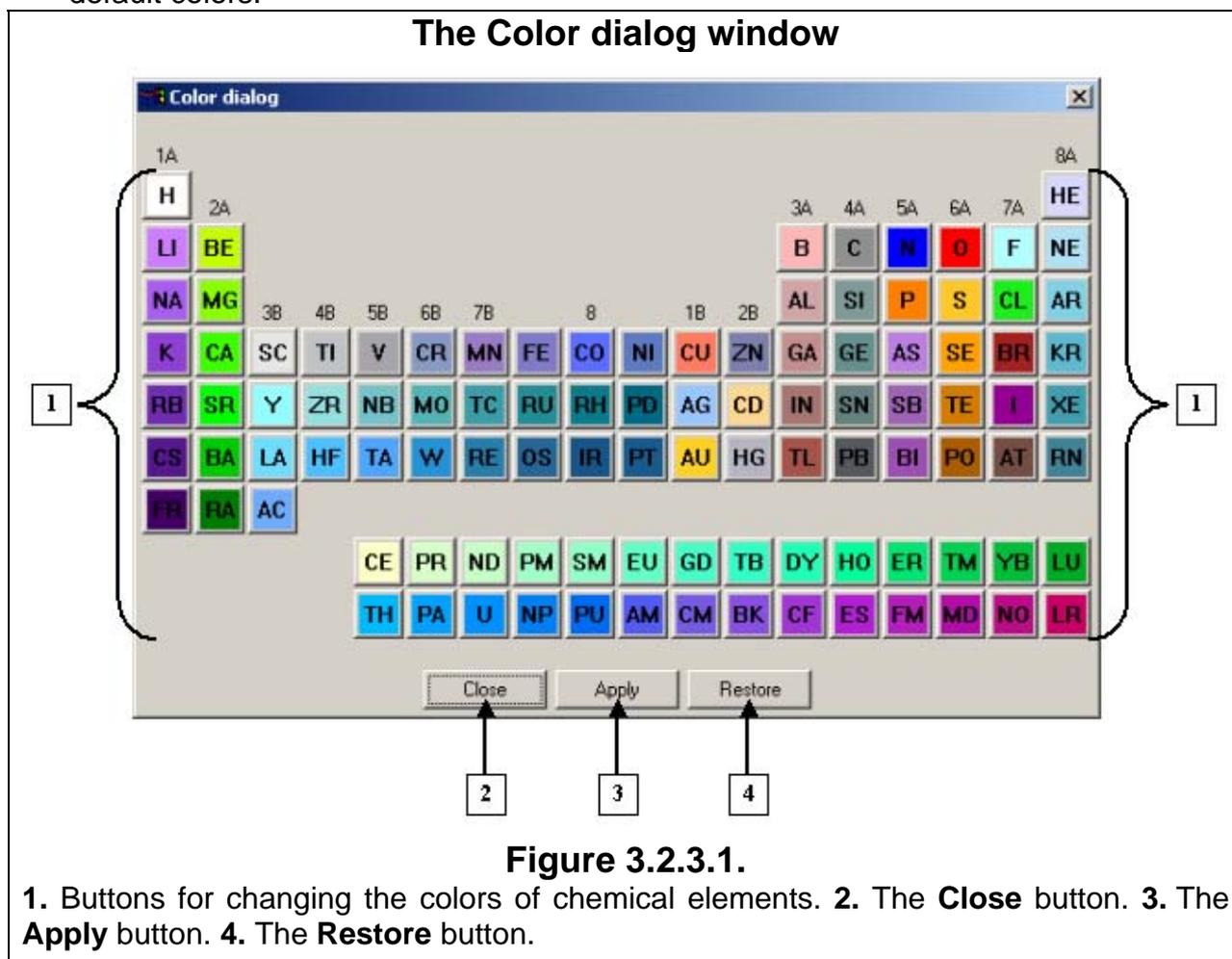
The Color dialog window contains colored buttons that are used to customize the colors of chemical elements. Each color corresponds to a certain element.

Click a colored button with the name of a chemical element to open a dialog window for this specific element, for example, "NITROGEN" (Fig. 3.2.3.2):

- The **Color** button shows the current color of the element. After you click this button, the **Color dialog window** will appear on your screen (see Section 3.9). In this dialog window, change the color of a chemical element. The **Color** button will change its color, too. Click **OK** to close the dialog window and apply changes. In the **Color dialog window**, 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 window and then click either the **Close** or **Apply** buttons in the **Color dialog window**, the model will be changed according to the new parameters.

Dialog window control buttons:

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



The NITROGEN dialog window

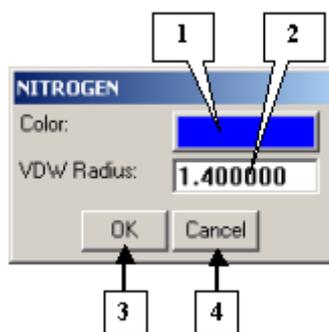


Figure 3.2.3.2.

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 window. 4. The **Cancel** button closes the dialog window and cancels changes.

3.3. Moving the model

3.3.1. Replacing 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.

3.3.2. Rotating the model

You can rotate the model using your mouse. The rotation speed is adjusted in the **Options** dialog window (see Section 3.7). 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 window. Select **View>Animation>Set delay** in the main menu to open this dialog window (Fig. 3.3.2.1). 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 window



Figure 3.3.2.1.

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

3.3.3. 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 window (see Section 3.7). If  button is pressed, a distance to selected elements of the scene only can be changed.

Comments. To load the initial image of the model, click the  toolbar button.

To make the model fit the view area, click the  toolbar button.

3.4. Selecting elements of the model

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.

Comment. Elements of models can also be selected using “Tree explorer” and “Sequence viewer” dialog windows (see chapter 3.5), as well as context menu of display area (see chapter 2.4.1.1)..

3.5. Lists of model elements

3.5.1. Hierarchical tree

The **Tree explorer** dialog window (Fig. 3.5.1.1) contains the hierarchical tree of the elements of a model that can be generated by:

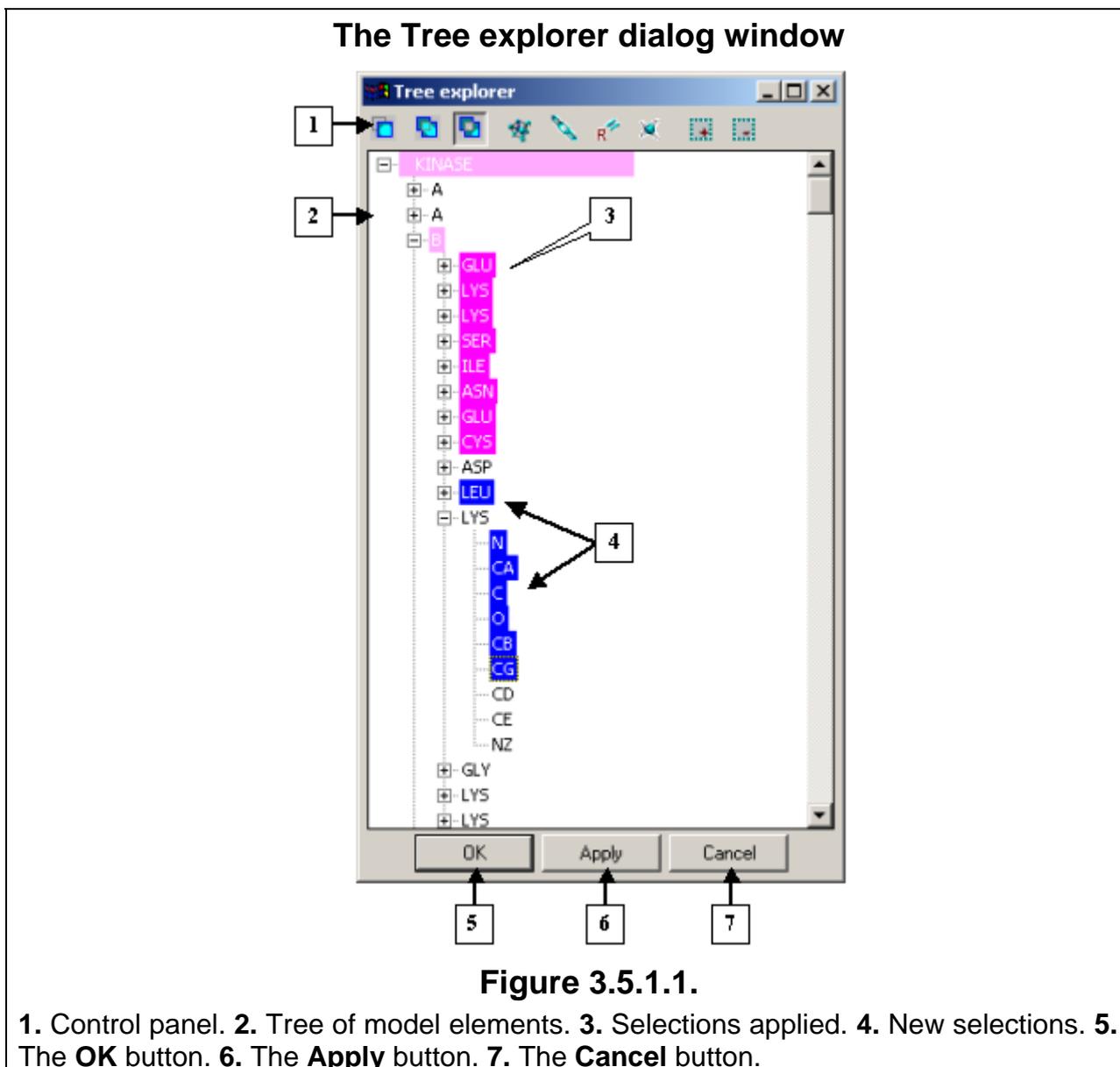
- Selecting the **Window>Tree dialog** option in the main menu.

Or:

- Clicking the  toolbar button.

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

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



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 window control buttons

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

3.5.2. Sequence viewer dialog window

You can open the **Sequence viewer** dialog window (Fig. 3.5.2.1) designed to view sequences of protein chains by:

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

3.5.2.1. Structure of the Sequence viewer dialog window

The **Sequence viewer** dialog window contains:

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

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 window (see Section 3.5.2.2) of the **Sequence viewer** dialog window.

The Sequence viewer dialog window

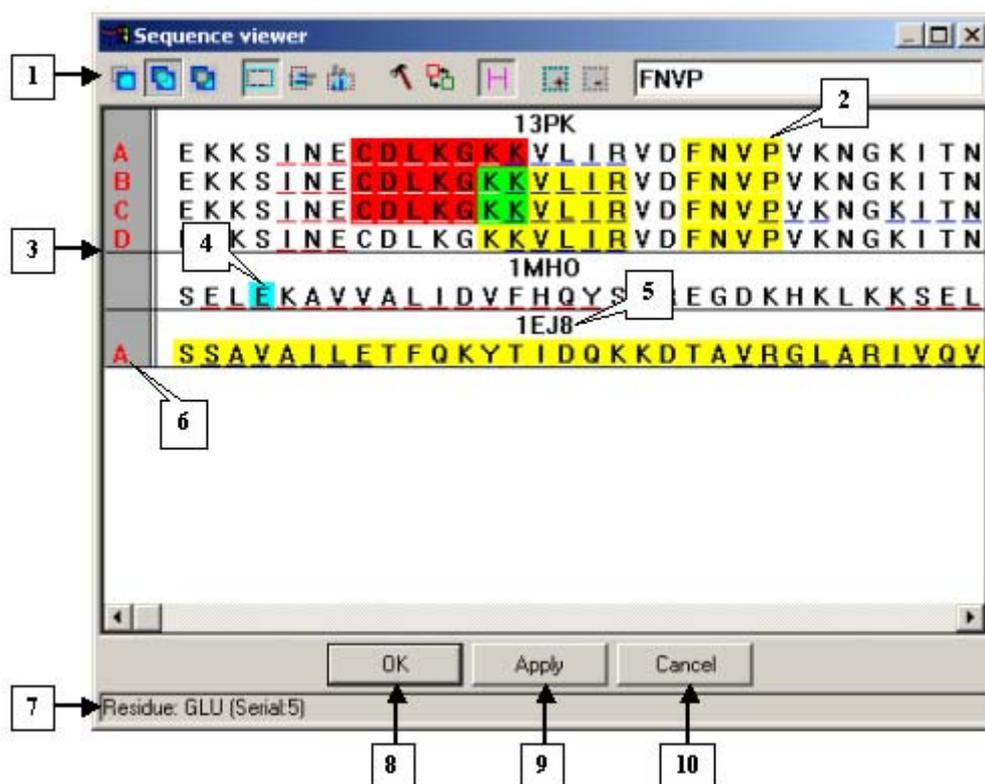


Figure 3.5.2.1.

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.

 – **Hide or show elements.** Click this button to open the **Visible and hidden elements** dialog window in which you can enable/disable some models to be displayed in the sequence view area (see Section 3.5.2.3).

 – **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 window 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 (Fig. 3.5.2.1).

Sequence view area

The sequence view area shows chain sequences in one-letter code (Fig. 3.5.2.1). You can select residues within this view area. In the **Options** dialog window (see Section 3.5.2.2), 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 window). The background color of chain names is customized in the **Options** dialog window. 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 (Fig. 3.5.2.1).

Dialog window control buttons:

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

Status bar

The status bar shows:

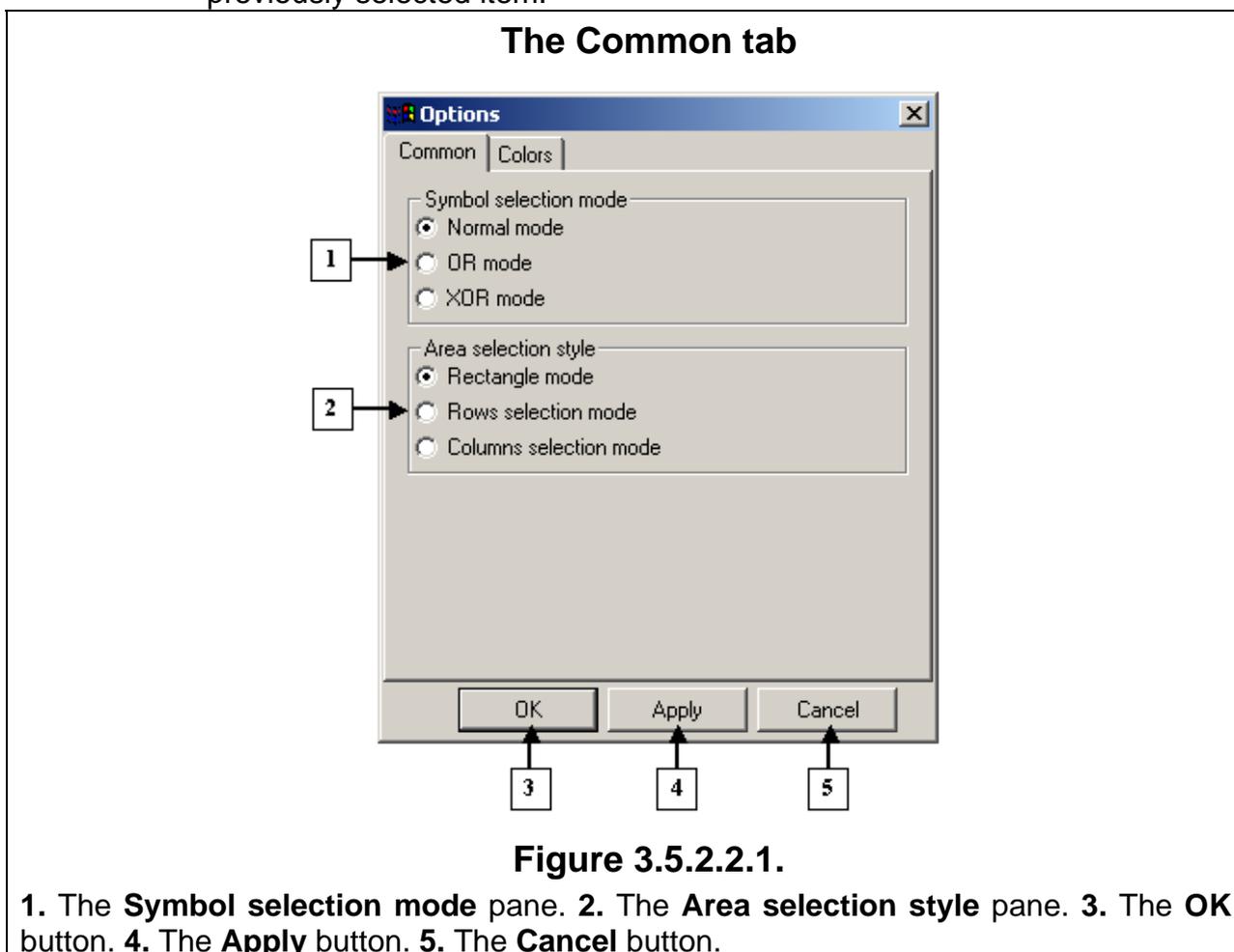
- Information about the residue you are pointing to with your mouse: residue name in three-letter code and its number in the PDB file (Fig. 3.5.2.1).
- The name of the control panel button you are pointing to with your mouse.

3.5.2.2. Options box of the Sequence viewer dialog window

To open the **Options** dialog window, click the  control panel button in the **Sequence viewer** dialog window. The **Options** box has two tabs: the **Common** tab (Fig. 3.5.2.2.1) which allows you to adjust selection modes for the **Sequence viewer** dialog window and the **Colors** tab (Fig. 3.5.2.2.2) which serves to customize the colors of selected residues.

Common tab

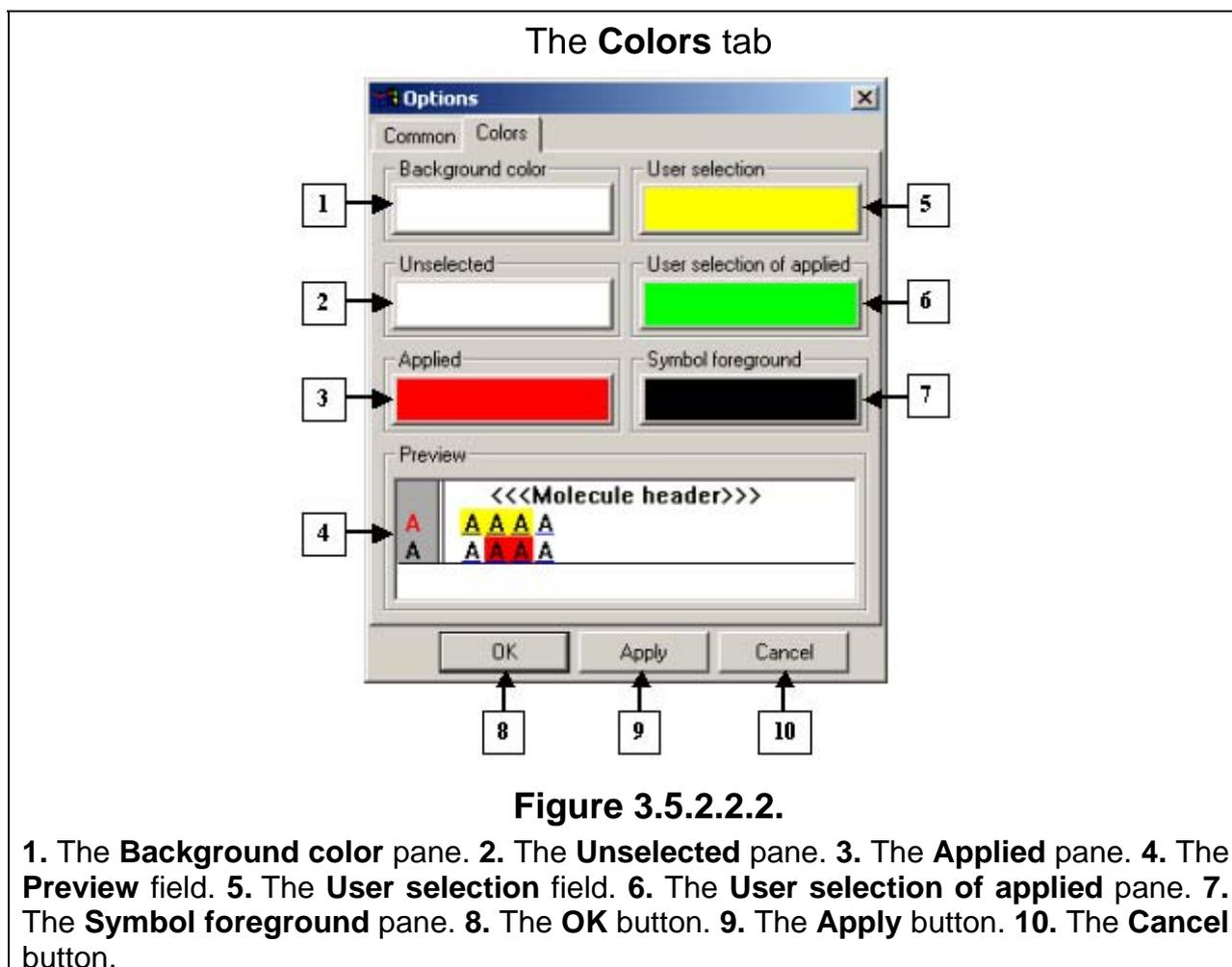
- On the **Symbol selection mode** pane, you can set the following selection modes:
 - **Normal mode** – In this mode, each subsequent selection unselects the previously selected item.



- **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

- 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 window appears on your screen. In this dialog window, you can select a background color (see Section 3.9 about the **Color** dialog window).



- 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 window appears on your screen. In this dialog window, you can

customize the color of unselected residues (see Section 3.9 about the **Color** dialog window).

- 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 window appears on your screen. In this dialog window, you can select a color for applied selections (see Section 3.9 about the **Color** dialog window).
- 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 window appears on your screen. In this dialog window, you can set a color for new selections (see Section 3.9 about the **Color** dialog window).
- 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 window appears on your screen. In this dialog window, you can select a color of these sections (see Section 3.9 about the **Color** dialog window).
- 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 window appears on your screen. In this dialog window, you can customize the color of symbols (see Section 3.9 about the **Color** dialog window).
- In the **Preview** field, you can preview the customized colors.

Dialog window control buttons:

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

3.5.2.3. Visible and hidden elements dialog window

To open the **Visible and hidden elements** dialog window (Fig. 3.5.2.3.1), click the  control panel button in the **Sequence viewer** dialog window. In the **Visible and hidden elements** dialog window, 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 window.

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.

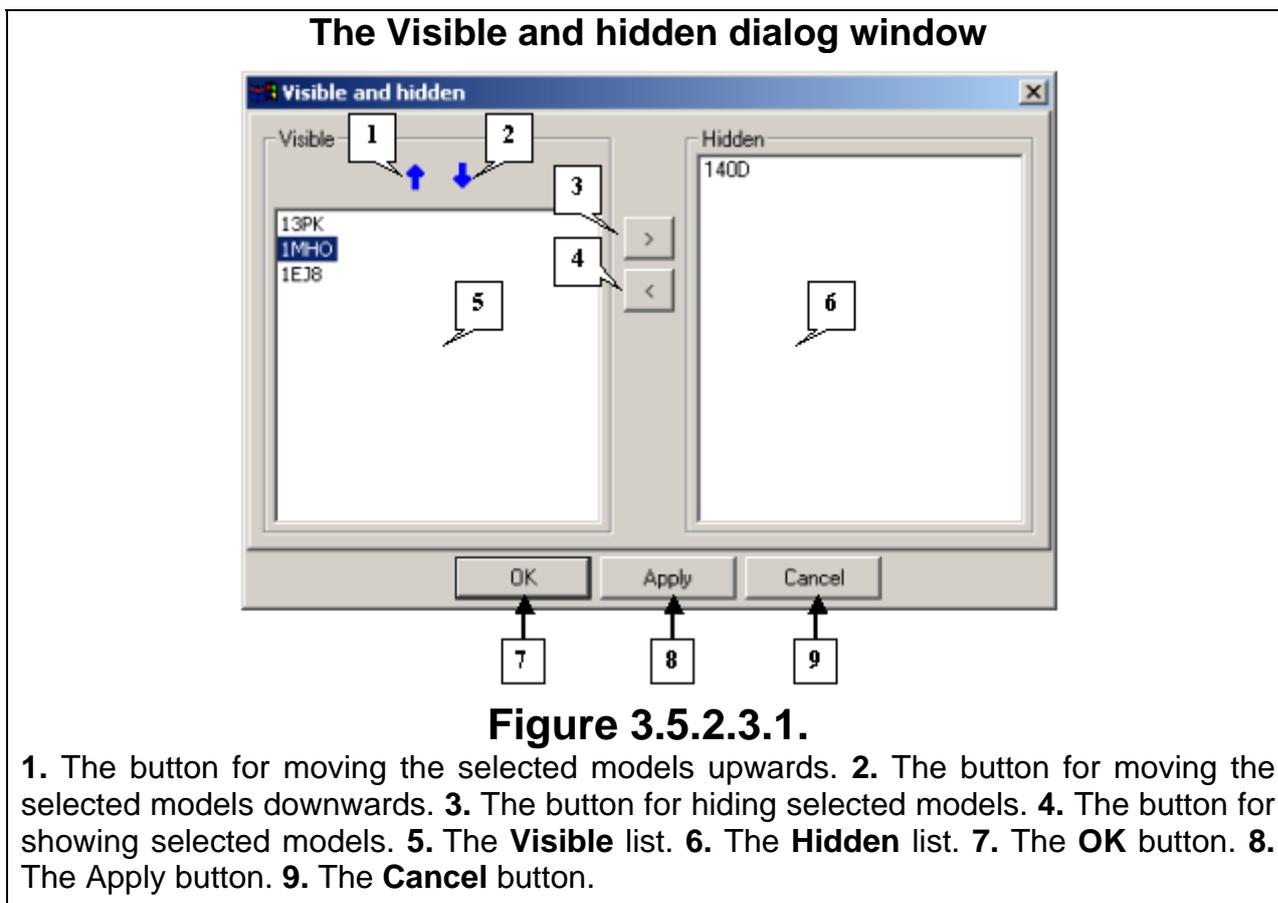
To hide some models, follow these steps:

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 below or above.

Dialog window control buttons:

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



3.6. Selecting scene elements to be displayed

You can select specific atoms, chains, residues, and chemical elements to be displayed in a model on the **Model options** dialog window (Fig. 3.6.1). To open this dialog window, do the following:

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

The information panel displays the following data about all loaded models and for the model selected in the drop-and-down list:

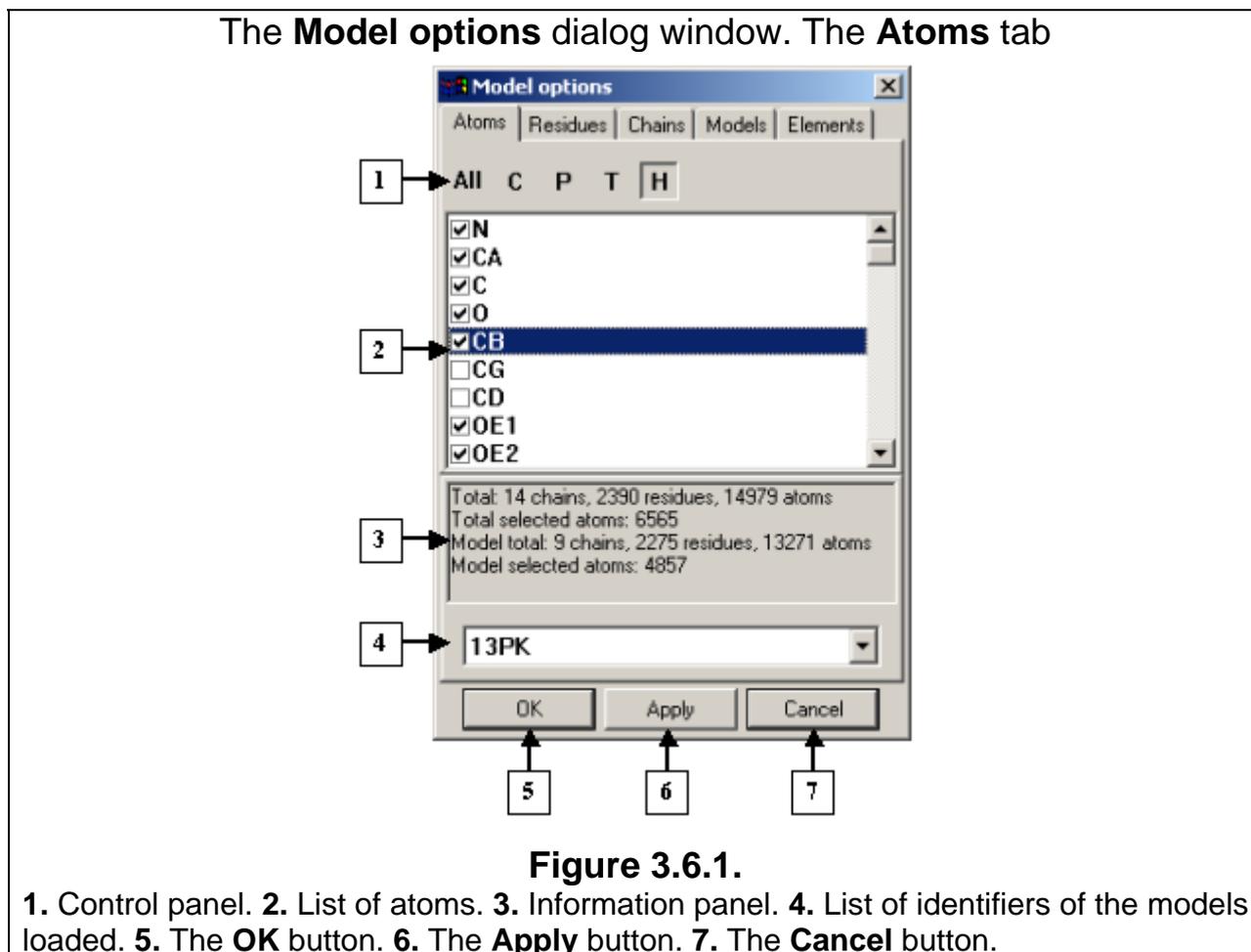
1. The total number of chains, residues, and atoms in models and the number of displayed atoms.
2. The number of selected atoms.

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: C α , N, C, and O.
- **P** – some of the protein backbone atoms: C α , N, and C.

- **T** – only C α - atoms in the protein backbone.
- **H** – all hydrogen atoms are hidden.



The **Residues** tab (Fig. 3.6.2) 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 window. The Residues tab

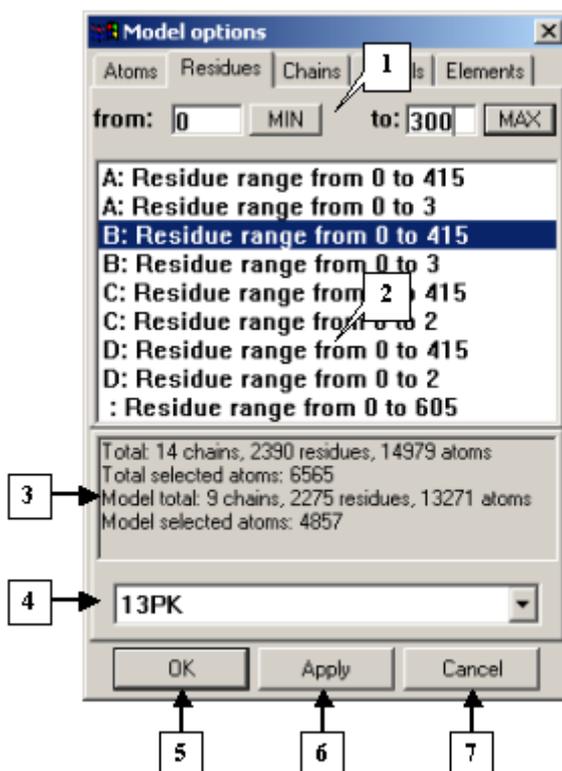


Figure 3.6.2.

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.

The Model options dialog window. The Chains tab

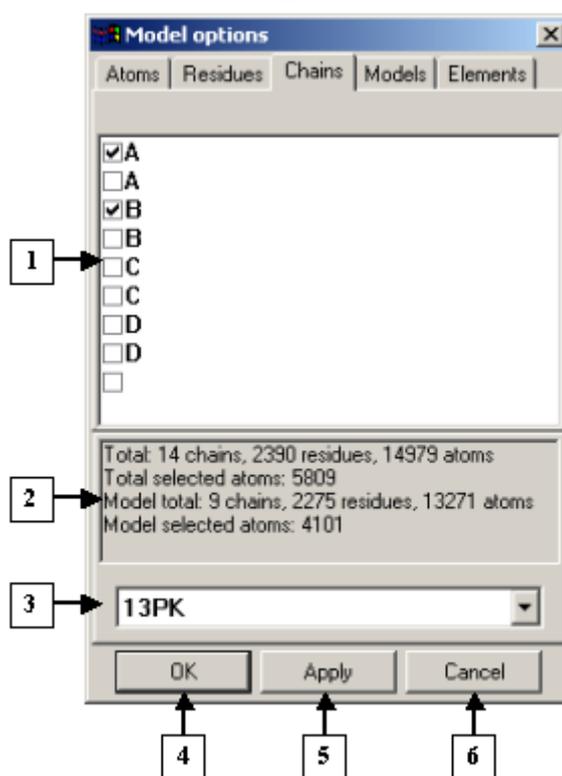


Figure 3.6.3.

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 **Elements** tab (Fig. 3.6.4) 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 window. The Elements tab

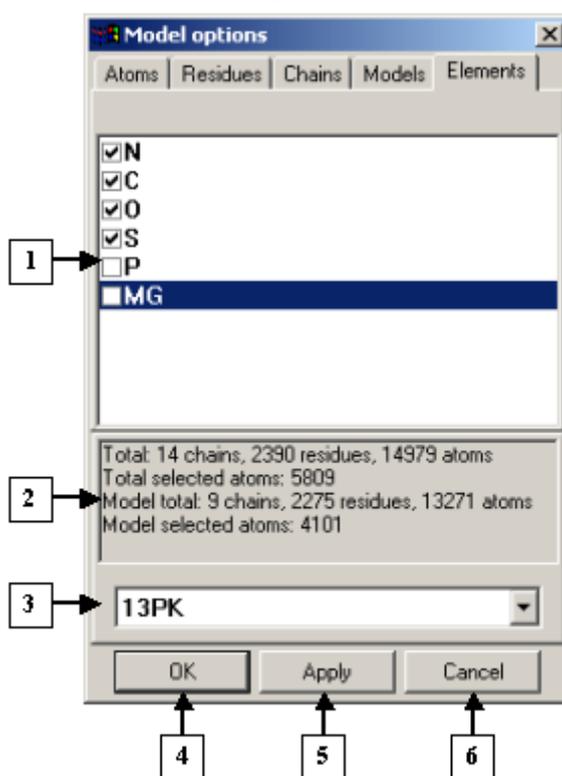


Figure 3.6.4.

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

The **Models** tab (Fig. 3.6.5) 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 window. The Models tab

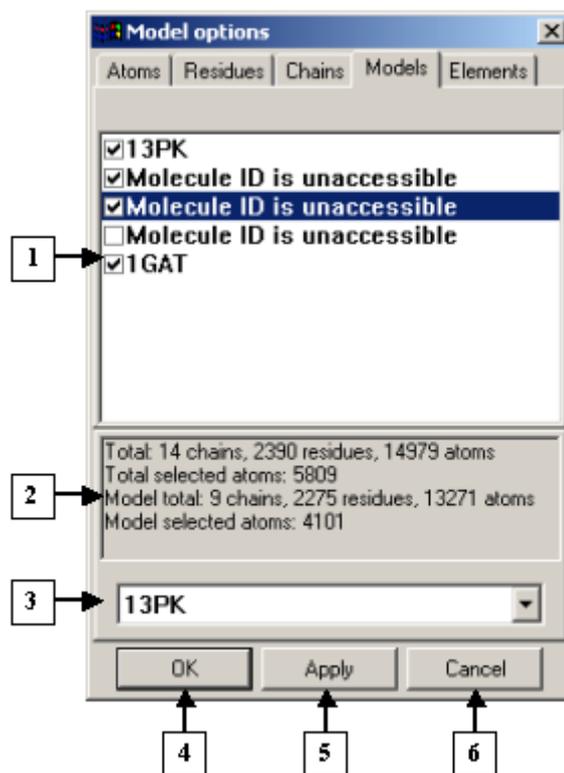


Figure 3.6.5.

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

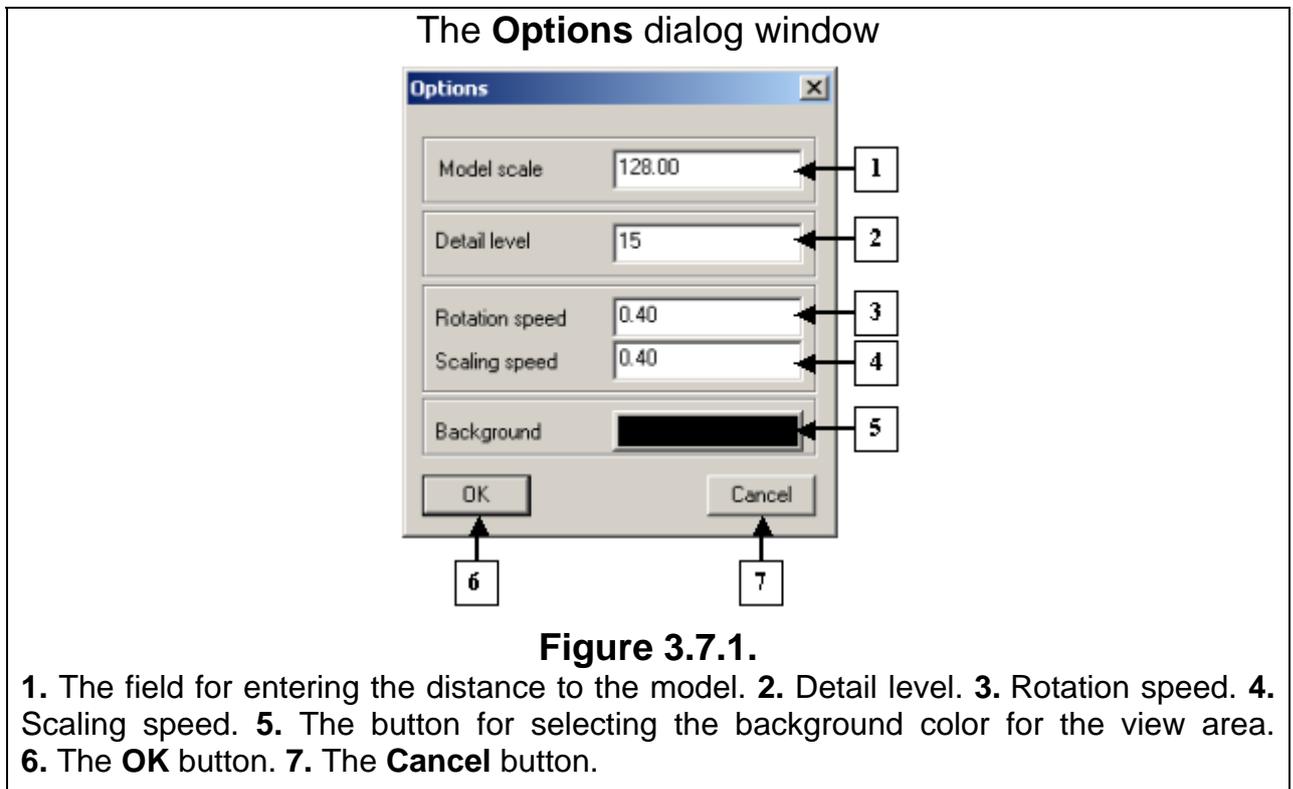
Dialog window control buttons:

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

3.7. Options dialog window

On the **Options** dialog window (Fig. 3.7.1), you can set the general parameters of the model and mouse parameters. To open the **Options** dialog window, do the following:

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



In the **Options** dialog window, 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 window and select a background color. See Section 3.9 about the **Color** dialog window.

Dialog window control buttons:

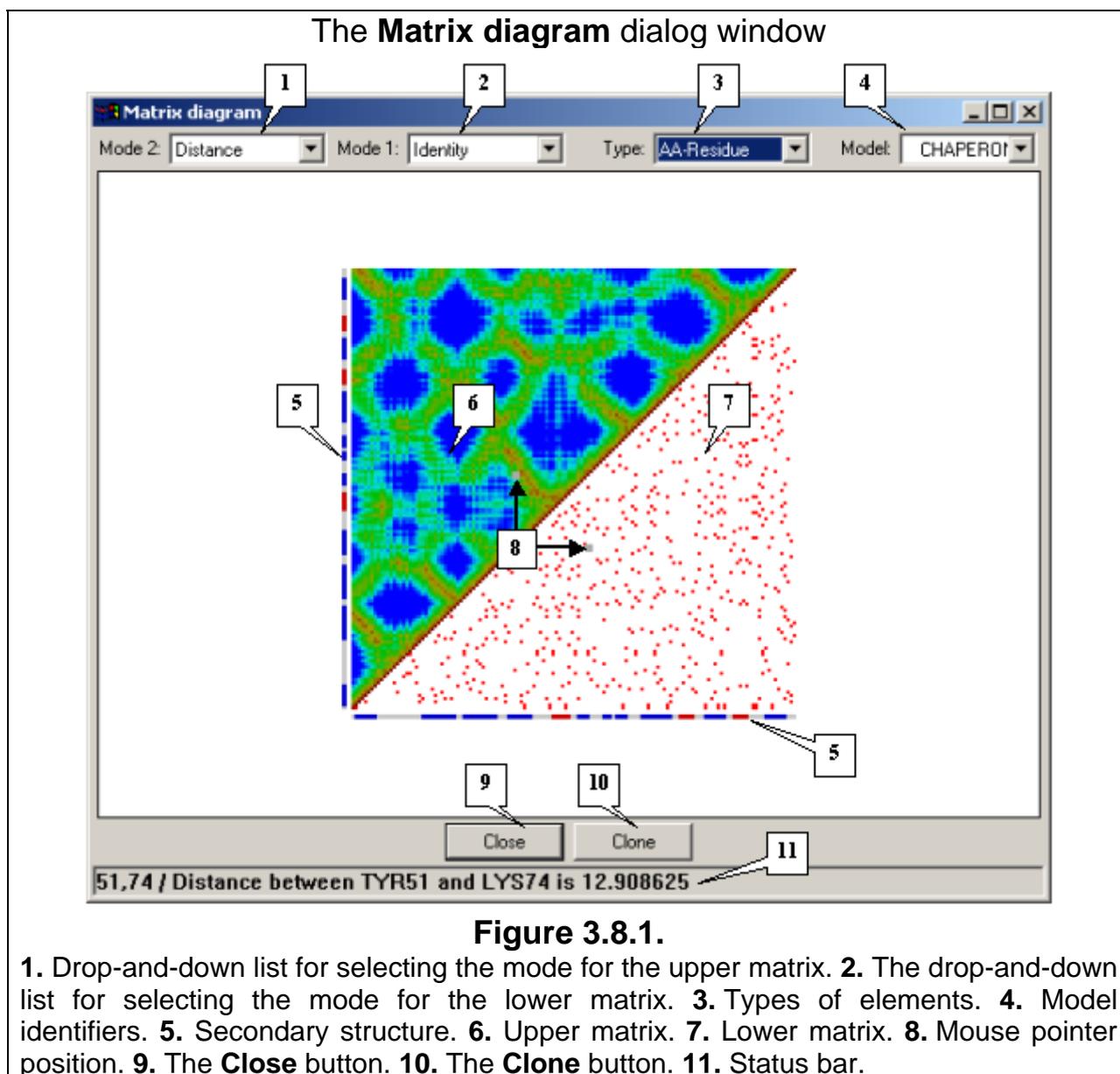
- Click **OK** to apply changes and close the dialog window.
- Click **Cancel** to cancel changes and close the dialog window.

3.8. Matrix diagram dialog window

In the **Matrix diagram** dialog window (Fig. 3.8.1), you can set the program to display structural features of models as matrix diagrams. To open the **Matrix diagram** dialog window, 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 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 window.

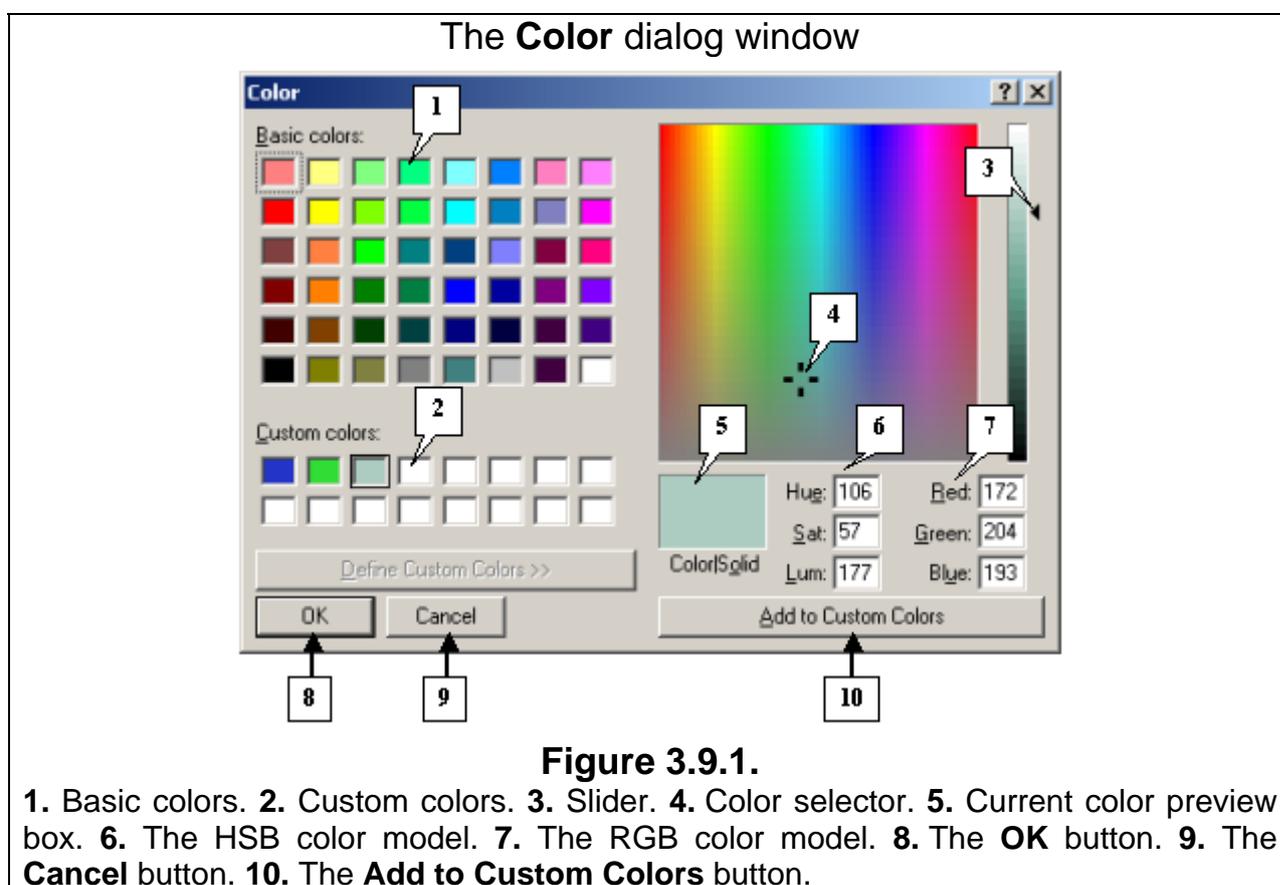
Click the **Close** button to close this dialog window.

3.9. Color dialog window

In the **Color** dialog window (Fig. 3.9.1), 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**.

Comment. 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 window control buttons

Click the **Apply color** button to apply changes and leave the dialog window open or click **OK** to apply changes and close the dialog window. Click the **Cancel** button to cancel changes.

4. References

1. www.rcsb.org/pdb/info.html#File_Formats_and_Standards
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

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