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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].

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.

1.1. Installation

1.1.1. Installing to Web-server

1. To switch to the folder with distributive
2. To compile the applet by the following sequence of commands:
 make clean
 make build
 make install
3. To copy jar-file into required directory of the web-server
4. To install «GetFile» program into cgi-bin folder of the Web-server

1.1.2. Installing to local computer

To install 3D-Explorer to local computer the following procedures are required:

1. To install JRE
2. To install Java3d RE
3. To copy jar-file into required user's directory

1.2. Starting Softberry 3D Explorer (Java version)

Softberry 3D Explorer Java version can be started by the following means:

1. Starting applet from the server with use of a certain HTML-code, inserted into html-page.
2. Starting application:
 - 2.1 Starting application for work with Web-server.
 - 2.2 Starting application for local work.

1.2.1. Starting the applet:

The following html-code should be inserted into html-page:

```
<APPLET      ARCHIVE="proteins.jar"      CODE="softberry.project.proteins.Base"
CODEBASE="/proteins/" WIDTH=10 HEIGHT=10>
<PARAM name="cgi" value="/cgi-bin/getfile">
<PARAM name="data_file" value="/var/www/tmp/java.KHgpna">
<PARAM name="help" value="/proteins/help/prot_hlp.html">
</APPLET>
```

Where:

ARCHIVE – name of the archive file with executable code of the applet.

CODE – basic class of the applet.

CODEBASE – catalog at the web-server with the archive of applet's executable code.

WIDTH – width of the applet on the internet-browser screen in pixels (it is not recommended to set it lesser than 10).

HEIGHT – height of the applet on the internet-browser screen in pixels (it is not recommended to set it lesser than 10).

PARAM – a certain parameter of the applet with following attributes:

name – name of a parameter.

value – value of a parameter.

Several parameters are allowed. There are essential for starting 3D-Explorer parameters:

1. name="cgi". A value for this parameter is the relative URL for cgi-bin file (data and query server). On incorrect definition of this parameter, the applet will not work.
2. name="data_file". A value for this parameter is the relative URL for file with data in special format (see chapter 1.3). On incorrect definition of this parameter, the applet will not work.
3. name="help". A value for this parameter is the relative URL for documentation file. On incorrect definition of this parameter, the applet will not work.

1.2.2. Starting the application

The common way for the application startup has the following appearance:

```
java -mx500 -cp "PATH_TO_JAR"proteins.jar softberry.project.proteins.Base  
[web options]
```

1.2.2.1. Starting the application for working with Web-server

Command for startup:

```
java -mx500 -cp "PATH_TO_JAR"proteins.jar softberry.project.proteins.Base [-c  
getatoms.cgi] [-get getfile.cgi] [-cce ce.cgi] [-sQH sQH.cgi] [-host host][  
-port port]
```

Value for parameter «**-host**» is defined by the Web-server, used for access to server application. This parameter is essential for working with Web-server.

Value for parameter «**-port**» is defined by the port, used for working with Web-server. This parameter is not essential. Default value is 80.

Value for parameter «**-c**» is defined by the relative URL for server application GetAtoms. The pathway to server application is defined in relation to Web-server. On incorrect definition of this parameter, the work with GetAtoms will be unavailable.

Value for parameter «**-get**» is defined by the relative URL for server application GetFile. The pathway to server application is defined in relation to Web-server. This is an essential parameter for work with Web-server.

1.2.2.1. Starting the application for local work

Command for startup:

```
java -mx500 -cp "PATH_TO_JAR"proteins.jar softberry.project.proteins.Base
```

1.2.3. Data formats for work with Web-server

1.2.3.1. Data format for downloading from server

STRUCTURE__

The list of structures can be empty. A single string corresponds to a single structure. A string has the following appearance:

```
file structureId
```

where:

file – name of the file with PDB data on the server (relatively to the root directory of the Web-server),

structureId – identifier of a structure

__STRUCTURE

ALIGNMENT__

The list of alignments can be empty. A single string corresponds to a single alignment. A string has the following appearance:

structure1 chain1 structure2 chain2 file

where:

structure1 – identifier of the first structure in alignment (must be the same as one in STRUCTURE block)

chain1 – strand for the first structure,

structure2 – identifier of the second structure in alignment (must be the same as one in STRUCTURE block)

chain2 – strand for the second structure,

file – name of the file with alignment on the server (relatively to the root directory of the Web-server) (description of the format see in chapter 1.3.2).

__ALIGNMENT

Example:

```
/*Example start here*/
STRUCTURE__
  /var/www/tmp/prot.CgqAd5 1hba
  /var/www/tmp/prot.CgqAd6 1hbb
__STRUCTURE
ALIGNMENT__
  1hba B 1hbb A /var/www/tmp/prot.CgqAd7
__ALIGNMENT
/*Example end here*/
```

1.2.3.2. Format of alignment

HEADER__

SOURCES__

FILE1: - file with the first structure

FILE2: - file with the second structure

CHAIN1: identifiers of the first strand

CHAIN2: identifiers of the second strand

SIZE1: length of the first strand (including gaps)

SIZE2: length of the second strand (including gaps)

__SOURCES

__HEADER

ALIGNMENT__

Strings of alignment in the following manner:

{Position on sequence1} {aligned sequence1 segment}

{Position on sequence2} {aligned sequence2 segment}

__ALIGNMENT

Example:

```
/*Example start here*/
HEADER__
SOURCES__
FILE1: /usr1/apache/tmp/cce.zjmRVT
FILE2: /usr1/apache/tmp/cce.cnHbQL
CHAIN1: B
CHAIN2: A
SIZE1: 146
SIZE2: 141
__SOURCES
```

```

__HEADER
ALIGNMENT__
2 HLTPEEKSAVTALWGKV--NVDEVGGEALGRLLVVYPRTQRFFESFGDLSTPDAVMGNPKVKAHGKKVLG
1 VLSPADKTNVKAAWGKVGAAHAGEYGAEALERMFSLFPTTKTYFPHFDL-----SHGSAQVKGHGKKVAD

70 AFSDGLAHL DNLKGT FATLSELHCDKLHVDPENFRLLGNVLCVLAHFGKEFTPPVQAAYQKVVAGVAN
65 ALTNAVAHVDDMPNALSALS D LHAHKL RVD PVNFKLLSHCLLVTLAAHLPAEFTPAVHASLDKFLASVST

140 ALAHKYH
135 VLTSKYR
__ALIGNMENT
/*****Example end here*****/

```

1.3. Loading the application

During the loading, on the main window background the information windows with reports on current loading and data processing steps (fig.1.3.1) appear.

If size of loading molecule exceeds the recommended one, then “Model options” dialog window appears. This window allows the number of displayed elements to be reduced (dialog description see in chapter 3.5 «Selecting the displayed elements of model»).

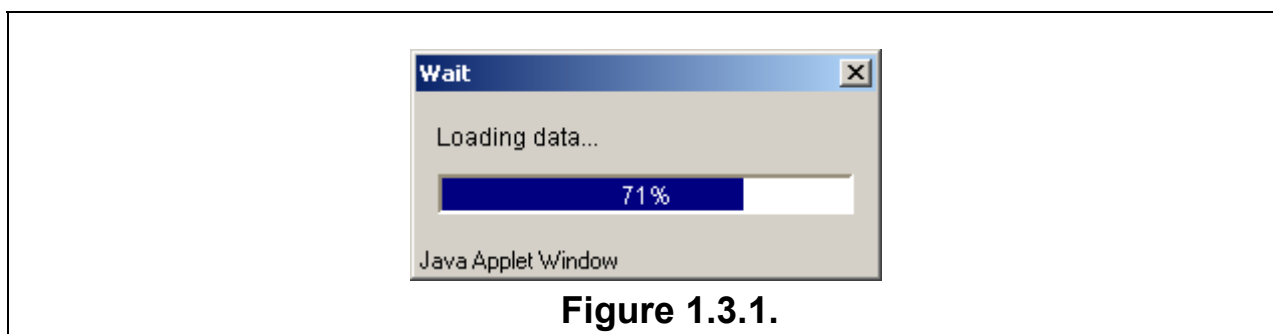


Figure 1.3.1.

1.4. Java3D Installation

Java3D Installation page 2 steps:

1) In order to run Java3D on your computer, you need to have Java SDK (or JRE) installed. For more information on installing Java, see [Sun's Java installation site](#). The instructions below concern Runtime Environment (RE) of Java3D only. If you want to download Java3D SDK, the procedures for downloading and installation are basically the same except that you have to choose SDK files instead of RE files. If you have installed the SDK, you have to install RE in order for Java3D function to function properly.

2) Install Java3D with DirectX or Java3D with openGL.

Operation System	Home page	Download from Softberry	Installation instruction
Windows	Sun Java3D site	Download	Sun installation instructions
Solaris	Sun Java3D site	Download	Sun installation instructions
Linux	Runtime Environment Blackdown Java3D site	Download	README file on Blackdown site

Windows

1) Download the appropriate Java3D runtime environment.

- 2) Run the executable by double-clicking on the file you downloaded. You can remove this file after installation.
- 3) You will also need DirectX and/or OpenGL installed on your computer.

Solaris

- 1) Download the appropriate Java3D runtime environment.
- 2) Run the executable. From the directory in which you installed Java3D, type the command:

```
java3d-1_2_1_01-solsparc-rt.bin
```

You can remove this file after installation.

Linux

- 1) Download Runtime Environment.
- 2) Move the file to the top level directory of the J2RE in which you wish to install Java3D, and go into this directory. Extract the file with:

```
bzip2 -dc ~/java3d-1.2.1_01-fcs-linux-i386-re.tar.bz2 | tar xvf -
```

- 3) After installation, you can remove the tar ball.
- 4) In order to run Java3D successfully, you should have one of the following system configuration:

- XFree86 3.3.6 with Mesa 3.1 or later
- XFree86 4.0.3 or later with XFree86's Mesa library and DRI
(*you can setup Mesa library from your Linux ditribution*)
- XFree86 4.0.3 with NVidia drivers 1.0-1251 or later
- XFree86 4.0.3 with an official (ie. not XFree86's) Mesa library (- see <http://www.mesa3d.org/>).

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
- Main view area
- Auxiliary view area
- Information panel
- Status bar

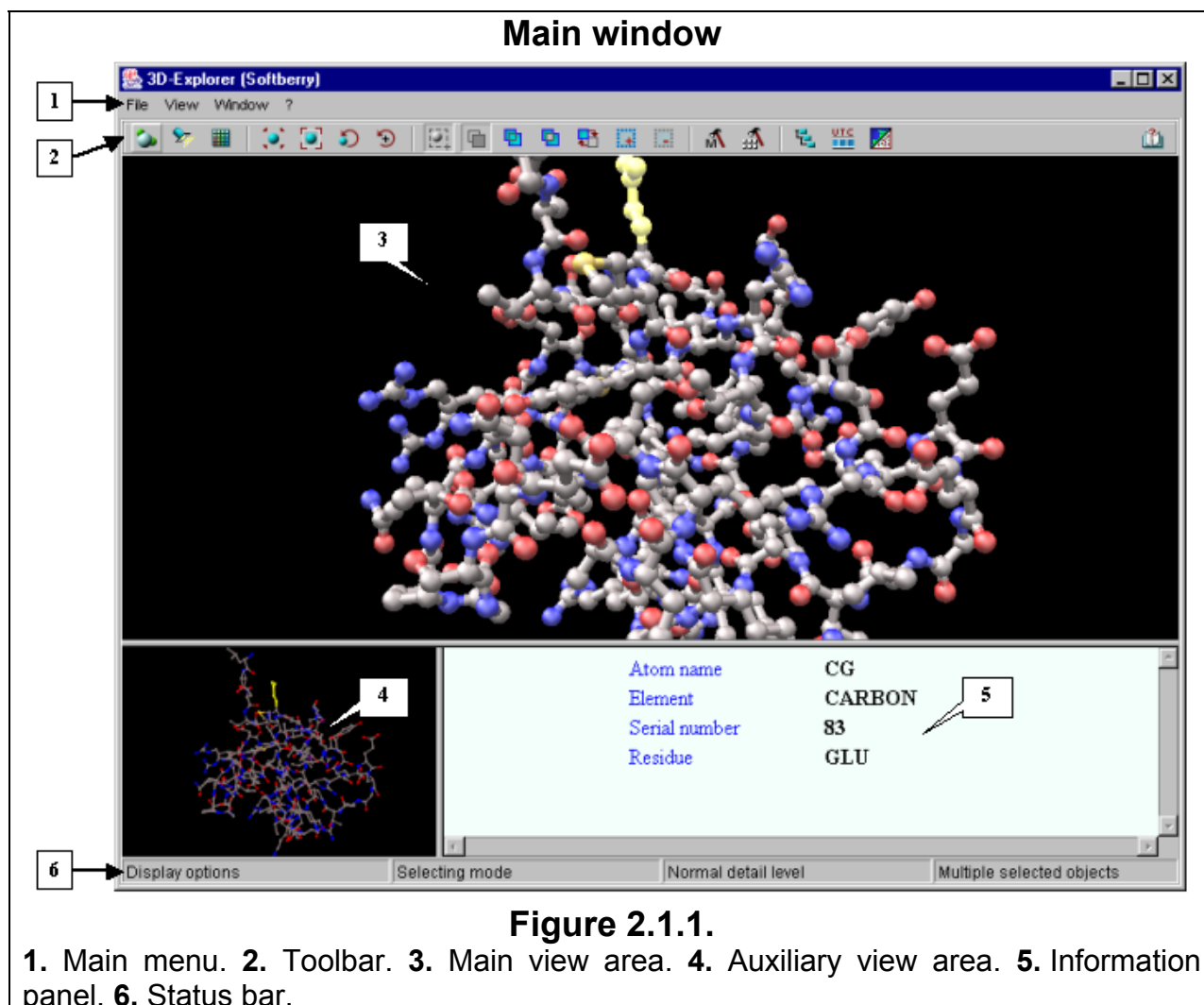


Figure 2.1.1.

1. Main menu. 2. Toolbar. 3. Main view area. 4. Auxiliary view area. 5. Information panel. 6. Status bar.

2.2. Main menu commands

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

- **Exit** – Quit the program.

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

- **Detail level** – Select the following detail levels for the model:
 - **Very low**
 - **Low**
 - **Normal**
 - **High**

- **Very high**
- **Custom** –user defined quality (this parameter is to be defined in «Options» dialog window, see Section 3.6).
- **Display style** – 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 **Periodic table** 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.

The **Window** menu has the following options:

- **Tree dialog** – Display the **Tree 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** dialog window to display specific features of the molecular structure as a matrix diagram.

The **?** menu has the commands:

- **Help** – Refer to Help Topics.
- **About** – Open the **About** dialog window with information about the program (Fig. 2.2.1).

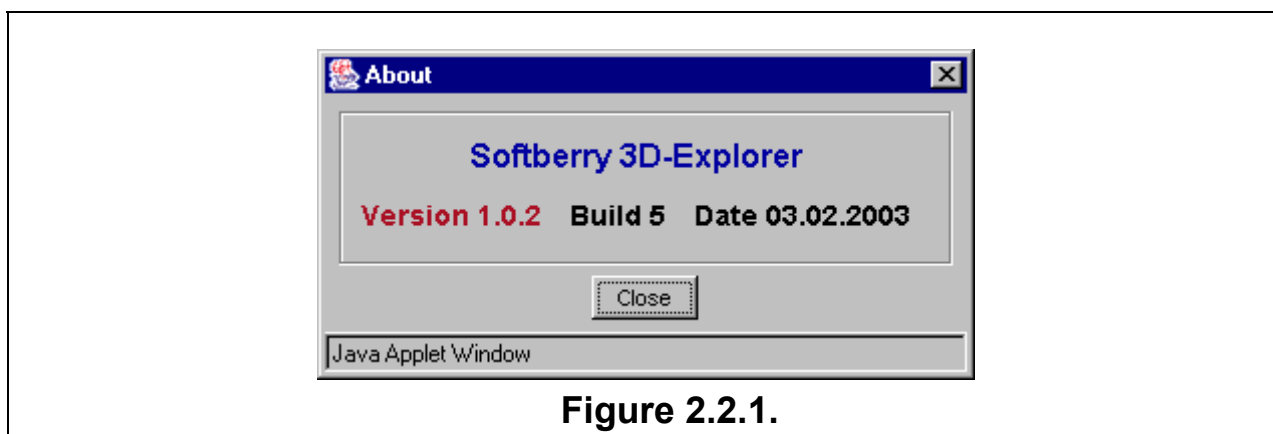






















Figure 2.2.1.

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 Periodic table dialog window to select colors for

	specific chemical elements. This button corresponds to the View>Colors menu command.
	Reset model position – Resets the initial model position.
	Fit model to screen – 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.
	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 viewer menu command.
	Matrix viewer – Open the Matrix dialog window to display specific features of the molecular structure as a matrix diagram. This button corresponds to the Window>Matrix dialog menu command.
	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. Model view areas

On the main area a model is displayed in selected display mode, on the auxiliary one – just in schematic view. The auxiliary area is purposed for changing a model's position as well as a distance to it. In the auxiliary area, the moving, rotating and changing a distance to model occur much quicker, that is very important at working with models, which contain a large number of atoms. Results of operations, performed on a model's image in the auxiliary area, are to be applied to model's image in the main area, and vice versa.

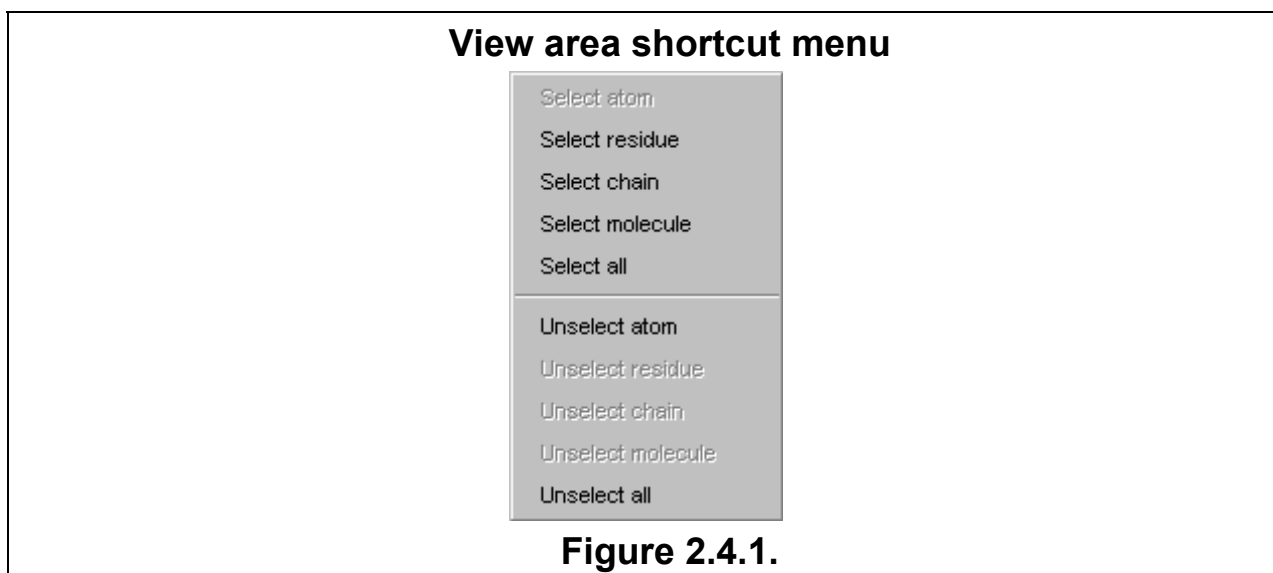
Use the **Options** dialog window to change the background color of the view area (see Section 3.6).

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), right-click the view area. The shortcut menu includes the following items:

- “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 molecule” – Select a molecule.
- “Select all” – Select all models.
- “Unselect atom” – Deselect an atom.
- “Unselect residue” – Deselect a residue.
- “Unselect chain” – Deselect a chain.
- “Unselect molecule” – Deselect a molecule.
- “Unselect all” – Deselect all models.



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.

2.6. Status bar

The status line (fig.2.1.1) is purposed for displaying current information. In this line, the function of control panel button, currently pointed by the mouse cursor, the current mouse operation mode, the current detailing level and the information on selection are displayed.

3. Working with the system

3.1. Working with images

3.1.1. Customizing image parameters


3.1.1.1. 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**
 - **Custom** – The quality set by the user (the given parameter is set in a dialogue window "Options", the description of dialogue see Section 3.6).
- Change the **Detail level** parameter in the **Options** dialog window (see Section 3.6).

3.1.1.2. Customizing the view

Display options dialog window can be opened by:

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

The **Display options** dialog window has two tabs: **Atom** and **Protein**. 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.

Tab *Atom*

Tab **Atom** (fig. 3.1.1.2.1) is used for setting up the displaying parameters for atoms of a model:

Display style panel provides the possibility to choose the view of a model or of a selected part of model:

- **Off** – To turn off the atoms' displaying.
- **Line** – The wire (skeletal) model. Bonds between atoms are shown as lines.
- **Stick** – The cylindrical model. Bonds between atoms are shown as cylinders. Diameter of cylinders is to be defined in **Stick size** field.
- **Ball and Stick** – The hinged model. Atoms are shown as spheres and bonds between atoms as cylinders. Diameter of cylinders is to be defined in **Stick size** field, and radius of spheres – in **Ball size** one.
- **CPK** – The complete atomic model (space-filling). Radiuses of spheres are proportional to van der Waals radiuses of atoms. The scale of spheres is to be defined in **CPK scale** field.

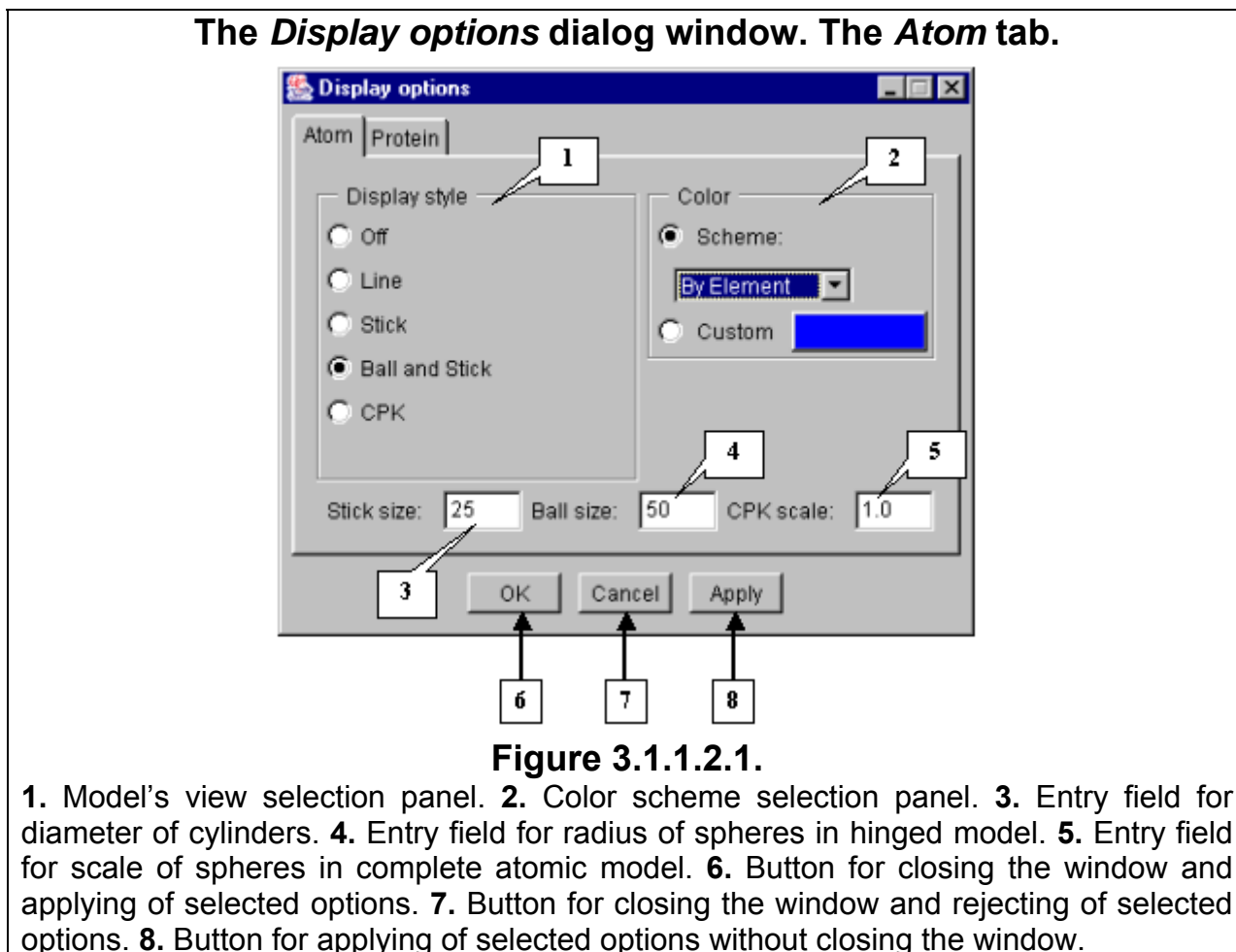
Color panel provides the possibility to choose the color scheme that is to be applied to atoms' view.

Upon selecting **Scheme** option, the list with following color schemes becomes active:

- **By Element** – The color of atom depends on chemical element.
- **By Chain** – The color of atom depends on chain it belongs to.

- **By Residue** – The color of atom depends on residue it belongs to. In this case, the term «residue» is applied to any group of covalently bound atoms (aminoacidic residues, nucleotides, heterogroups).
- **By Amino Acid** – The color of atom depends on amino acid it belongs to.
- **By Structure** – The color of atom depends on structure it belongs to.
- **By Groups** – The color of atom depends on its belonging to either main protein strand or side ones.

Upon selecting **Custom** option, the color button purposed for choosing the user-defined color of model or selected part of model becomes active. Upon pressing this button, **Color dialog** window (see chapter 3.7), in which a desired color can be chosen, appears.



Tab *Protein*

Tab **Protein** (fig. 3.1.1.2.2) provides the possibility to set up the parameters of model's displaying that are specific for protein molecule. Options of **Protein** tab can be applied to whole chain only.

Comment. If among the selected elements of a model there is at least one whole chain then tab is active. If not all daughter elements of a chain are selected (i.e. chain is selected just partially) then "Protein" tab is inactive. If one chain is selected completely, but another one – just partially then tab's options will be applied to the completely selected chain only.

Display style panel provides the possibility to choose the style of strands' displaying:

- **Off** – To turn off the displaying. Upon selecting this option, chains stops to be displayed.
- **CA Wire** – $C\alpha$ -atoms along the chain are bound by lines.
- **CA Stick** – $C\alpha$ -atoms along the chain are bound by cylinders. Diameter of cylinders is to be defined in **Stick size** field.
- **Line ribbon** – The protein molecule is shown as lines corresponding to the main chain direction.
- **Flat ribbon** – The protein molecule is shown as flat ribbon corresponding to the main chain direction.
- **Solid ribbon** – The protein molecule is shown as volumetric ribbon corresponding to the main chain direction.
- **Schematic** – The structure of molecule is shown in accordance to the following rules: α -helices are shown as wide cylinders, β -folds as arrows, bends and unknown structures as narrow cylinders (pipes).

The *Display options* dialog window. The *Protein* tab.

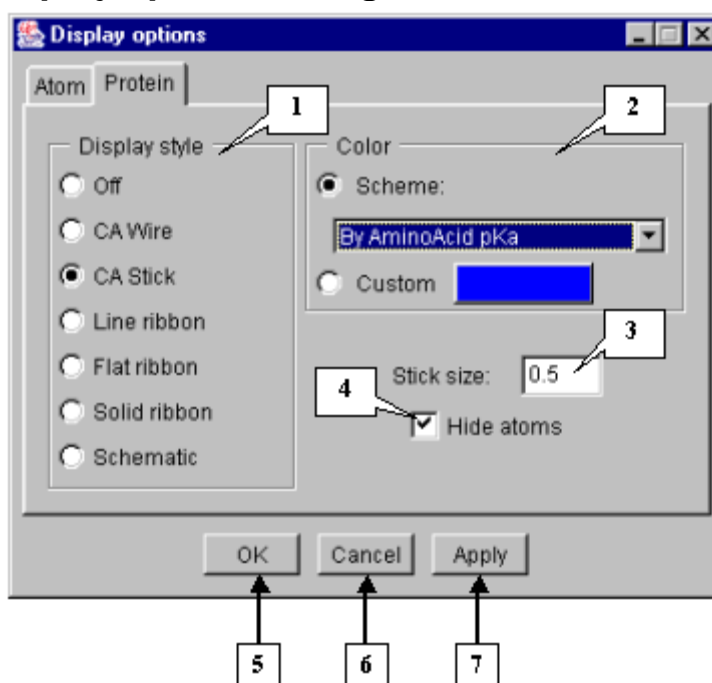


Figure 3.1.1.2.2.

1. Panel for selecting the protein chain view style. 2. Panel for selecting the color scheme. 3. Entry field for cylinder's diameter definition in "CA Stick" option. 4. Checkbox for turning off the model's atoms displaying. 5. Button for closing the window and applying of selected options. 6. Button for closing the window and rejecting of selected options. 7. Button for applying of selected options without closing the window.

Color panel provides the possibility to choose the color scheme to be applied to chains' view.

Upon selecting **Scheme** option the list with following color schemes becomes active:

- **By Chain** – every chain has its own color.
- **By Residue** – The color of chain's part depends on color of residue. In this case, the term «residue» is applied to any group of covalently bound atoms (aminoacidic residues, nucleotides, heterogroups).

- **By Amino Acid** – The color of chain's part depends on color of amino acid.
- **By Amino Acid Hydrophobicity** – The color of chain's part depends on its hydrophobic properties.
- **By Amino Acid pKa** – The color of chain's part depends on pKa value of amino acid.
- **By Structure** – The color of chain's part depends on structure it belongs to.
- **By Secondary structure** – The color of chain's part depends on its secondary structure. α -helices are shown in red color, β -folds in blue color, bends and unstructured parts in white one.

Comment. On **Flat ribbon** and **Solid ribbon** modes selecting, **By Secondary structure** color scheme is being set automatically.

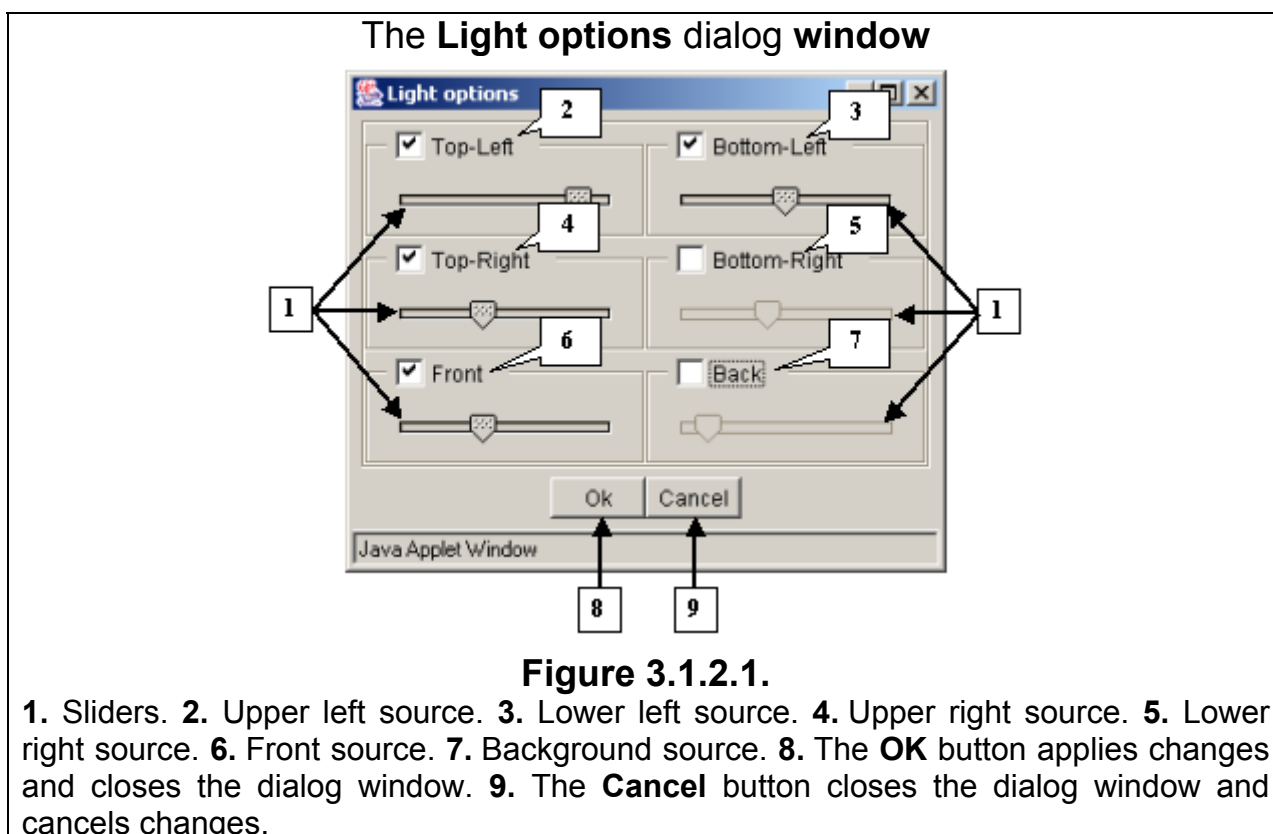
On **Custom** mode selecting, the colored button, purposed for choosing the user-defined color of a model, becomes active. Upon pressing this button, **Color dialog** window (see chapter 3.7), in which a desired color can be chosen, appears.


Hide atoms checkbox. If checkbox checked in, the model's atoms displaying is off.

Comment. Button **OK** is purposed for closing the window and applying the selected options, button **Apply** - for applying the selected options without closing the window, button **Cancel** - for closing the window and rejecting of selected options.

3.1.2. Light options

To open the **Light options** dialog window (Fig. 3.1.2.1), 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:

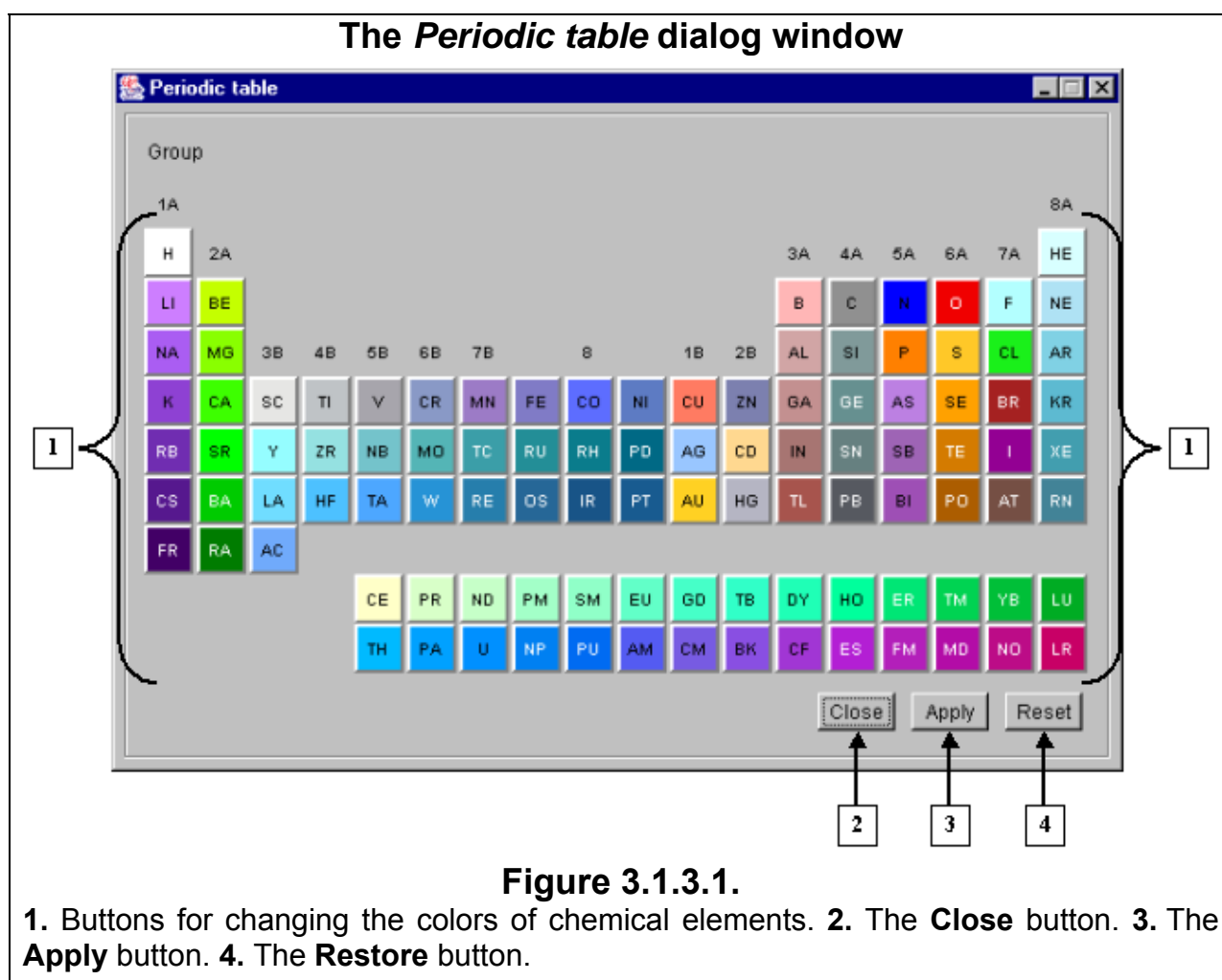
- **Top-Left** – the light source is placed on the left above the model.

- **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.

3.1.3. Selecting colors of chemical elements

You can change the colors of chemical elements in the **Periodic Table** dialog window (Fig. 3.1.3.1). To open this dialog box:

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



The **Periodic table** 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. 3.1.3.2):

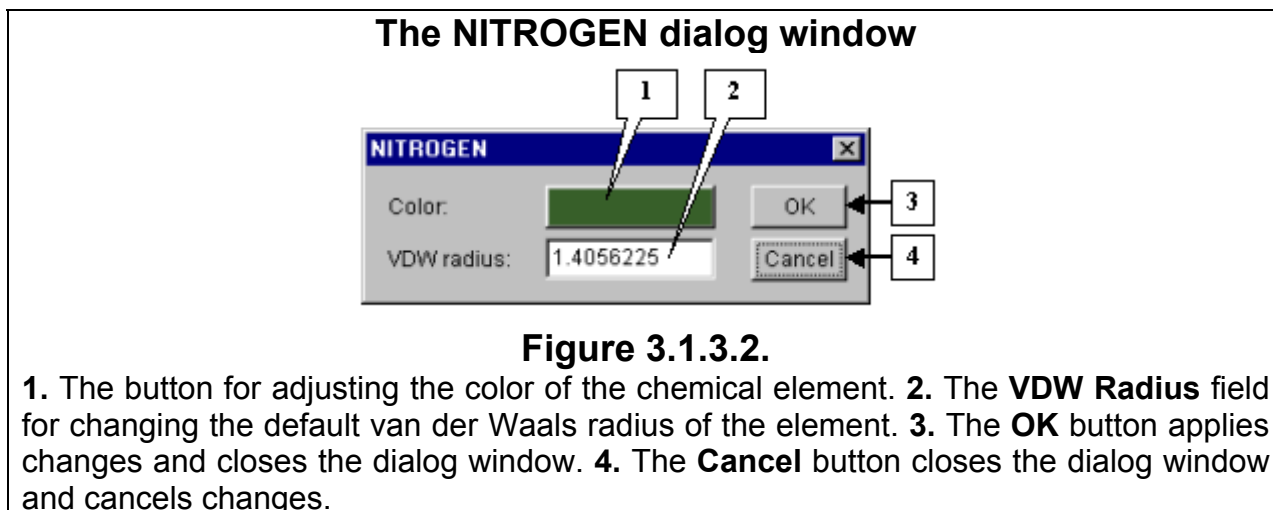
- The **Color** button shows the current color of the element. After you click this button, the **Color dialog** window will appear on your screen (see Section 3.9). In this dialog window, change the color of a chemical element. The **Color** button will change its color, too. Click **OK** to close the dialog box and apply changes. In the **Periodic table**

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 **Periodic table** 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 box window.
- **Restore** – Reset the default values of the van der Waals radii of the elements and default colors.



3.2. Model motions



3.2.1. 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.

3.2.2. Rotating the model


You can rotate the model using your mouse. The rotation speed is adjusted in the **Options** dialog window (see Section 3.6).


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.


3.2.3. 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 3.6).


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.


3.3. 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. The elements of models can also be selected using the **Tree dialog** and **Sequence viewer** dialog windows (see Section 3.4).

3.4. Lists of model elements

3.4.1. Hierarchical tree

The **Tree dialog** window (Fig. 3.4.1.1) 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.
- 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



– 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.



– 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.



- Invert a selection.



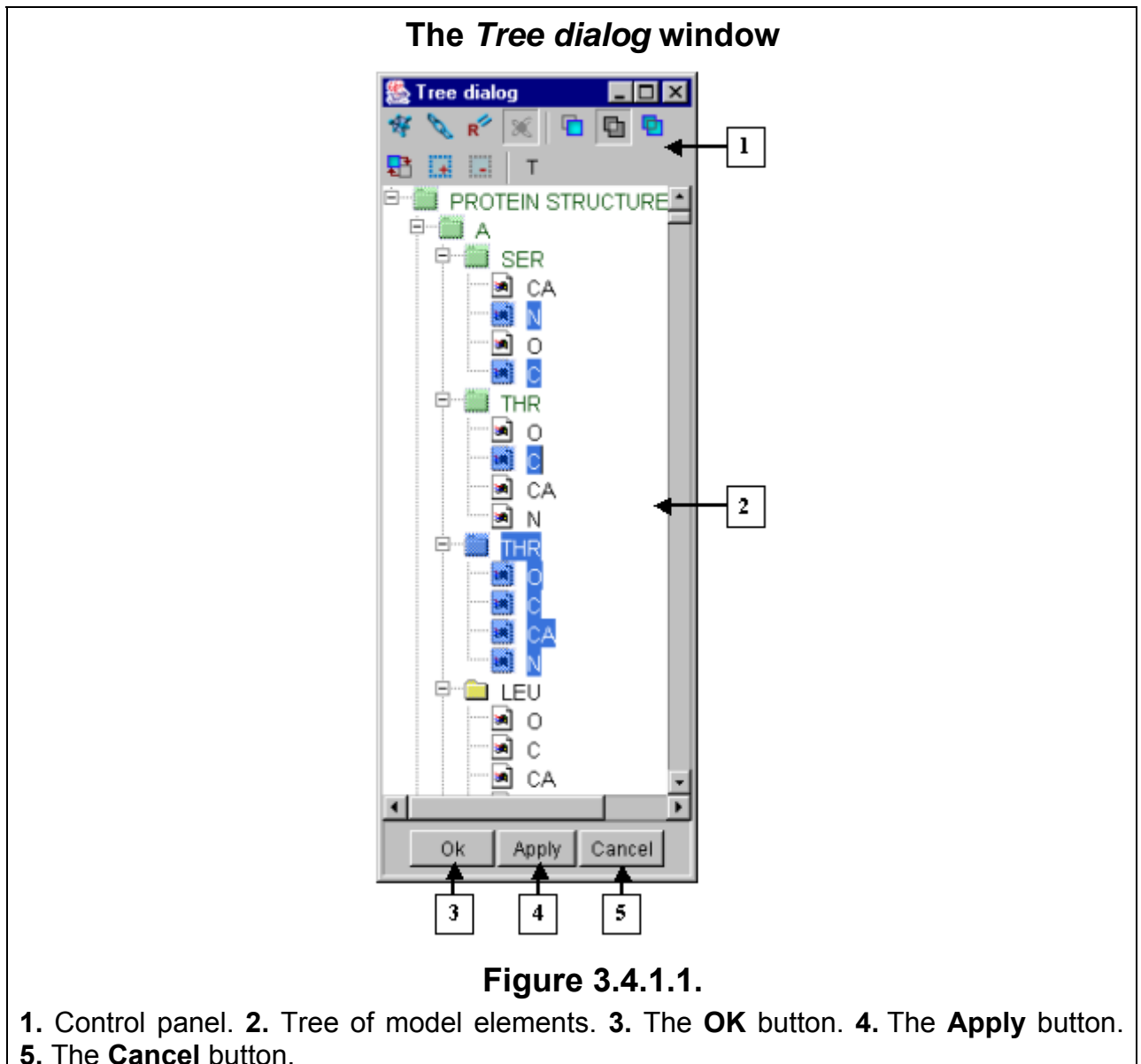
- Select all elements in the tree.



- Unselect all elements in the tree.



- When button is pressed, selecting of elements becomes immediately applied to model's displaying in display areas, and **Apply** and **Cancel** buttons becomes inactive. If button is released, selecting becomes applied on pressing **OK** or **Apply** buttons only



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.

Junctions containing at least one selected daughter element are marked in green.


Selected elements are marked in blue. If all daughter elements of a junction are selected, then this junction is also marked in blue. If junction is selected, its daughter elements are marked in blue.

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.

3.4.2. Sequence viewer dialog window

You can open the **Sequence viewer** dialog window (Fig. 3.4.2.1) designed to view sequences of protein chains by:

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

3.4.2.1. Structure of the Sequence viewer dialog window

The **Sequence viewer** dialog window contains:

- Control panel
- Sequence view area
- Dialog box 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 3.4.2.2) of the **Sequence viewer** dialog window.



– **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 3.4.2.3).



– **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 box there is an input field **Sequence** 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. 3.4.2.1).

Sequence view area

The sequence view area shows chain sequences in one-letter code (Fig. 3.4.2.1). You can select residues within this view area. In the **Options** dialog window (see Section 3.4.2.2), 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. 3.4.2.1).

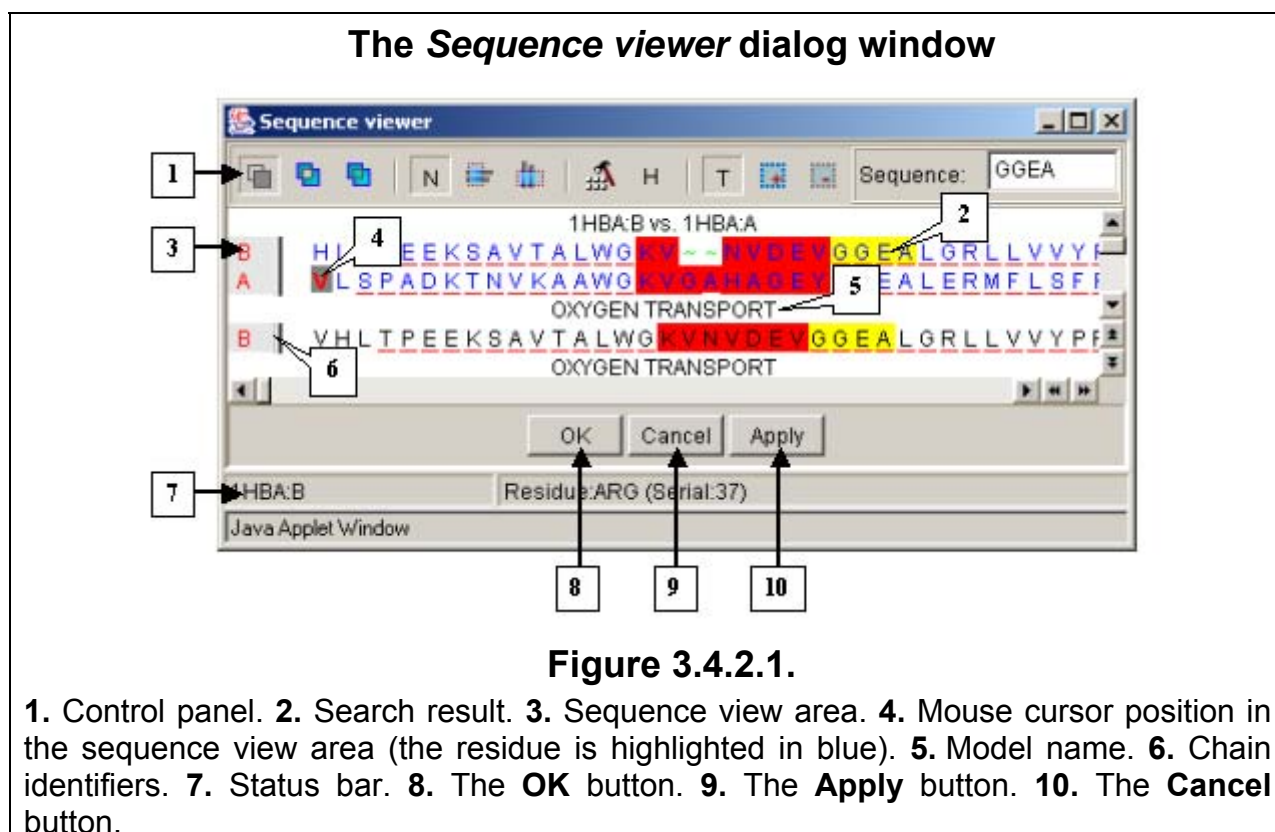


Figure 3.4.2.1.

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.

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. 3.4.2.1).

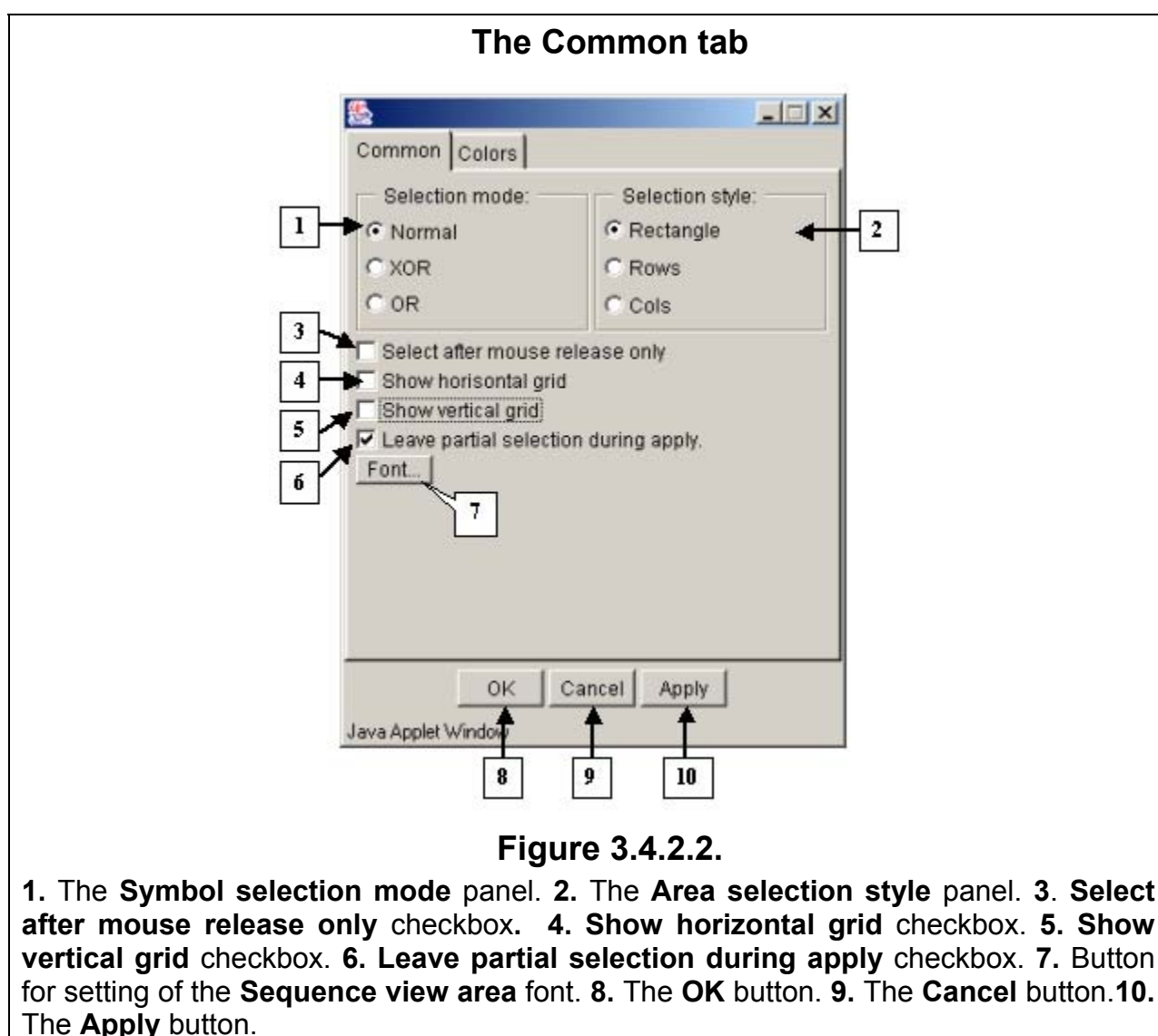
3.4.2.2. Options window of the Sequence viewer dialog window

Dialog window elements

To open the **Options** dialog window, click the  control panel button in the **Sequence viewer** dialog window. The **Options** window has two tabs: the **Common** tab (Fig. 3.4.2.2.1) which allows you to adjust selection modes for the **Sequence viewer** dialog window and the **Colors** tab (Fig. 3.4.2.2.2) which serves to customize the colors of selected residues.

Common tab

- On the **Symbol selection mode** panel, 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** panel, 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.
- Checkbox **Apply immediately**. If checkbox checked in, selection becomes applied to a model immediately after releasing the mouse button. If checkbox checked out, selection becomes applied on pressing **OK** or **Apply** buttons of **Sequence viewer** dialog window only.
- Checkbox **Select after mouse release only**. Not active in the current version.
- Checkbox **Show horizontal grid**. If checkbox checked in, then in area of amino acid sequences visualization the horizontal separator lines are shown (fig. 3.4.2.1). If checkbox checked out, the horizontal separator lines are not shown.
- Checkbox **Show vertical grid**. If checkbox checked in, then in area of amino acid sequences visualization the vertical separator lines are shown (fig. 3.4.2.1). If checkbox checked out, the vertical separator lines are not shown.
- Checkbox **Leave partial selection during apply**. If checkbox checked in, then partial selection of amino acids is being kept on applying a new one.
- Button **Font** is purposed for choosing a font of chains' and aminoacidic sequences' names. On pressing this button, **Font** dialog window, purposed for choosing a font (see chapter 3.9), appears.

Colors tab

- On the **Background color** panel, 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 3.7 about the **Color dialog** window).
- On the **Applied selection color** panel, 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 box, you can select a color for applied selections (see Section 3.7 about the **Color dialog** window).
- Panel **Partial selection** is purposed for choosing a color of residue that is selected partially (i.e. not all of atoms of residue are selected). The color of button corresponds to current color. On pressing the button, **Color dialog** window for color choosing appears. Operating this window is described in chapter 3.7.
- On the **Chain background** panel, you can select a background color for the names of the chains. 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 box, you can select a background color (see Section 3.7 about the **Color dialog** window).
- On the **User selection color** panel, 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 select a color for applied selections (see Section 3.7 about the **Color dialog** window).
- On the **Selection of applied** panel, 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 box, you can select a color for applied selections (see Section 3.7 about the **Color dialog** window).

The Colors tab

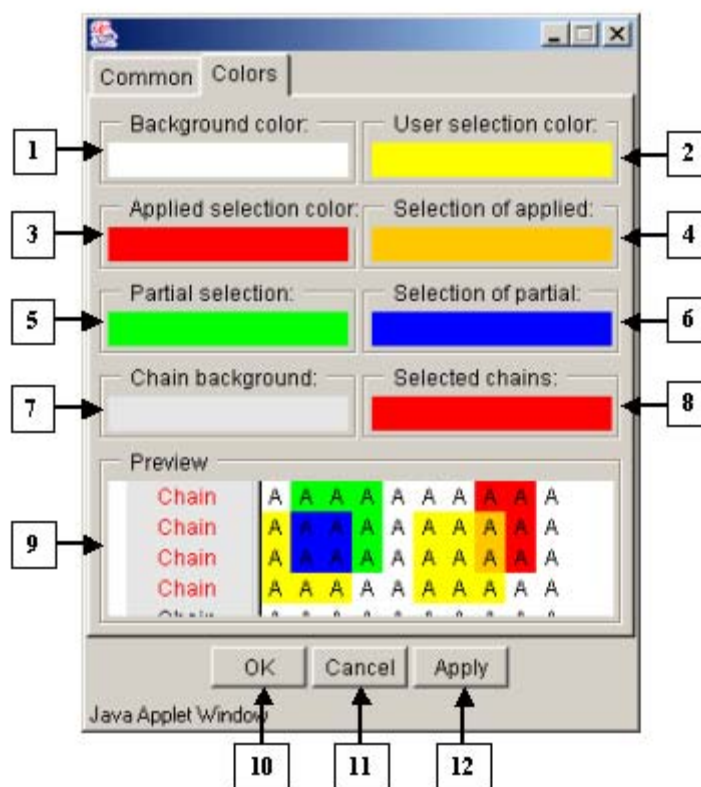


Figure 3.4.2.3.

1. The **Background color** panel. 2. The **User selection color** panel. 3. The **Applied selection color** panel. 4. The **Selection of allied** panel. 5. The **Partial selection** panel. 6. The **Selection of partial** panel. 7. The **Chain background** panel. 8. The **Selected chains** panel. 9. The **Preview** field. 5. The **User selection field**. 6. The **User selection of applied** panel. 7. The **Symbol foreground** panel. 10. The **OK** button. 11. The **Cancel** button. 12. The **Apply** button.

- Panel **Selection of partial** is purposed for choosing a color of residue that belongs to overlapping of partial and new selections. The color of button corresponds to current color. On pressing the button, **Color dialog** window for color choosing appears. Operating this window is described in chapter 3.7.
- Panel **Selected chains** is purposed for choosing a color of names of chains, containing the selected residues. The color of button corresponds to current color. On pressing the button, **Color dialog** window for color choosing appears. Operating this window is described in chapter 3.7.
- 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.

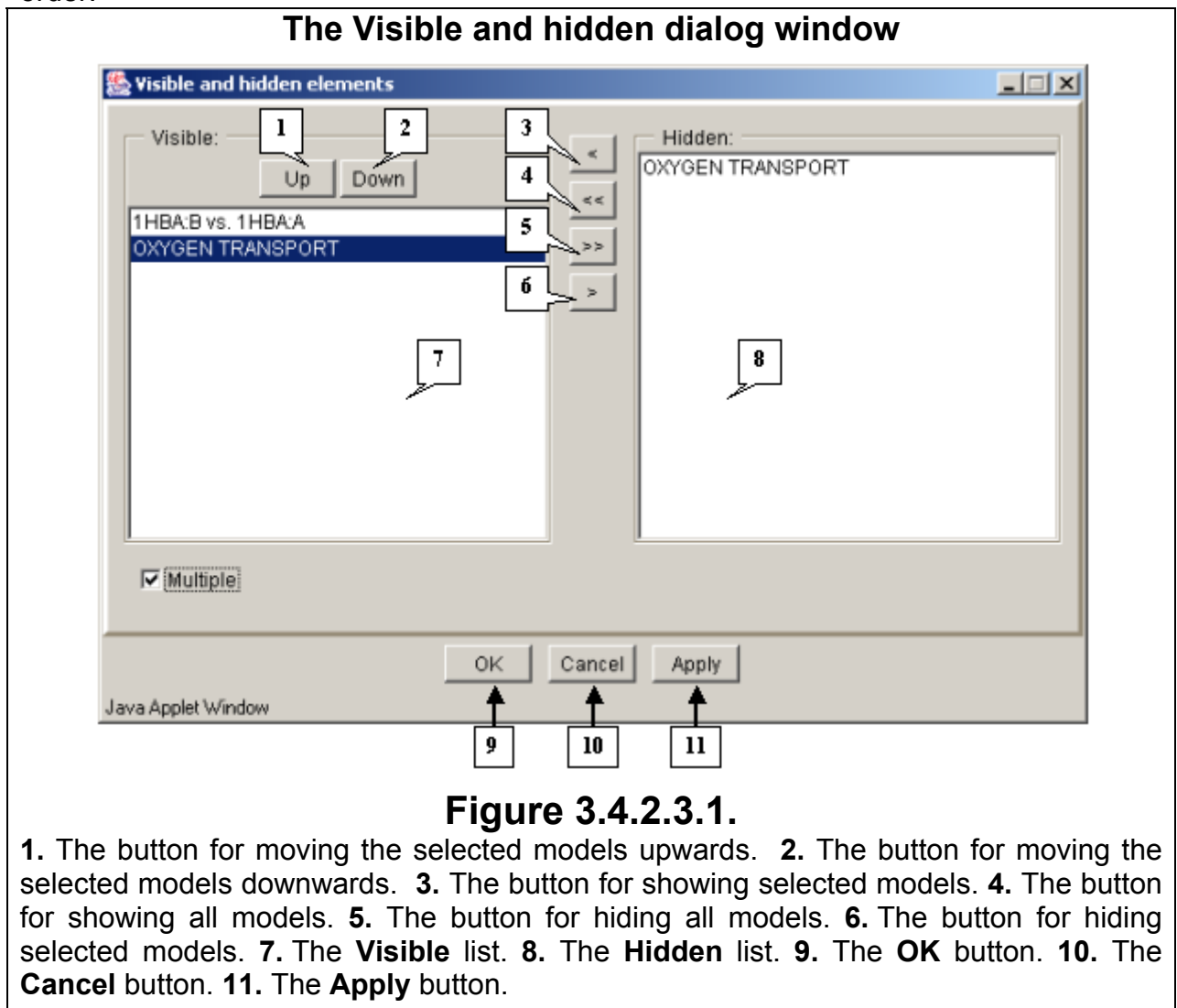
3.4.2.3. Visible and hidden elements dialog window

To open the **Visible and hidden elements** dialog window (Fig. 3.4.2.3.1), click the **H** 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 include all models (and alignments) in displaying it is necessary to press  button. All identifiers will be removed from «Hidden» list to «Visible» one in the same order.



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 exclude all models (and alignments) from displaying it is necessary to press  button. All identifiers will be removed from «Visible» list to «Hidden» one in the same order.


To change the order of models in the lists, click the **Up** or **Down** 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.

3.5. Selection of elements to be displayed

Atoms, strands, residues and chemical elements can be selected for displaying by using **Model options** dialog window (fig.3.5.1), which can be opened by one of the following means:

- Using **View>Model options** command of the main menu.
- Using  button on the control panel.

In the information bar the current information on all loaded models as well as on the model selected in the dropdown list is displayed:

1. Total numbers of strands, residues and atoms contained in models and a number of atoms included in displaying.
2. Number of atoms selected for displaying.

The list of models' identifiers is purposed for selecting a model, for which the display parameters can be changed.

The panel **Proteins** is purposed for selection of protein elements that are to be displayed:

Checkbox **Protein backbone**. If the checkbox checked in, the protein main chain is displayed. The chain displaying styles:

- **Trace** – only $C\alpha$ -atoms of a protein are selected.
- **Partial** – a part of the protein main chain's atoms are selected: $C\alpha$, N and C.
- **Complete** – all atoms of the protein main chain are selected: $C\alpha$, N, C and O.

Checkbox **Protein sidechains**. If the checkbox checked in, the protein sidechains are displayed.

The panel **DNA** is purposed for selection of DNA elements that are to be displayed:

Checkbox **Nucleotide backbone**. If the checkbox checked in, the sugar-phosphate chain of DNA is displayed.

Checkbox **Nucleotide bases**. If the checkbox checked in, the nucleotide bases are displayed.

Checkbox **Solvents**. If the checkbox checked in, the solvent's atoms are displayed.

Checkbox **Heterogenes**. If the checkbox checked in, the heteroatoms are displayed.

Buttons **Atoms**, **Chains**, **Residues**, **Elements** and **Models** call the appropriate dialog windows with lists of displayed atoms, chains, residues, chemical elements and models (fig.3.5.2).

The Model options dialog window

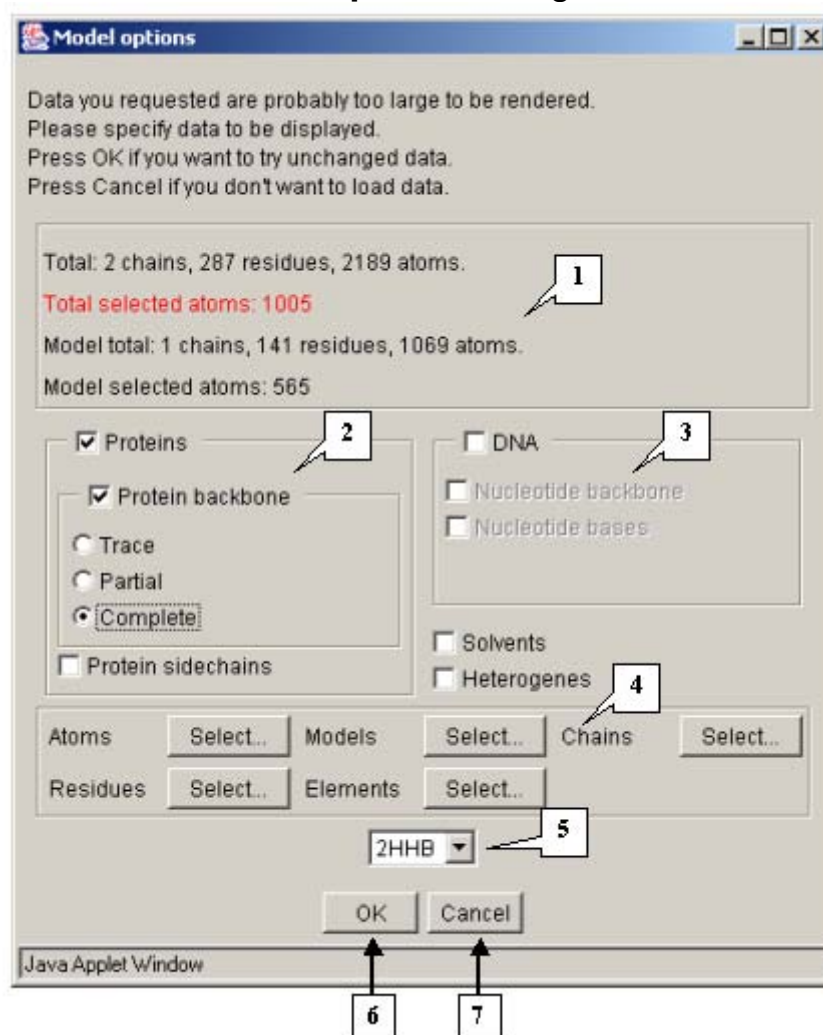


Figure 3.5.1.

1. Information bar. 2. Panel for selection of protein elements that are to be displayed. 3. Panel for selection of DNA elements that are to be displayed. 4. Panel for opening the lists of displayed elements of a model. 5. List of loaded models. 6. Button for closing the window and confirmation of the choice. 7. Button for closing the window and refusing of the choice.

In **Atoms**, **Chains** and **Models** dialog windows (3.5.2 A, C, D, E) it is necessary to select elements or models to be displayed. For these purposes, click the mouse button over a status indicator, which is located to the left of name of element. If a black square appeared on indicator (■), then element is selected for displaying, otherwise (□), it is excluded from displaying (fig.3.5.2).

In the **Atoms** dialog window, the buttons of the control panel above the list allow to include into displaying the following groups of atoms:

- The button **All** – all atoms in the list.
- The button **C** – atoms of the main protein chain: C α , N, C and O.
- The button **P** – the part of atoms of the main protein chain: C α , N, and C.
- The button **T** – C α - atoms of the main protein chain only.

- The button **H** – pressing of the button excludes the hydrogen atoms from displaying.

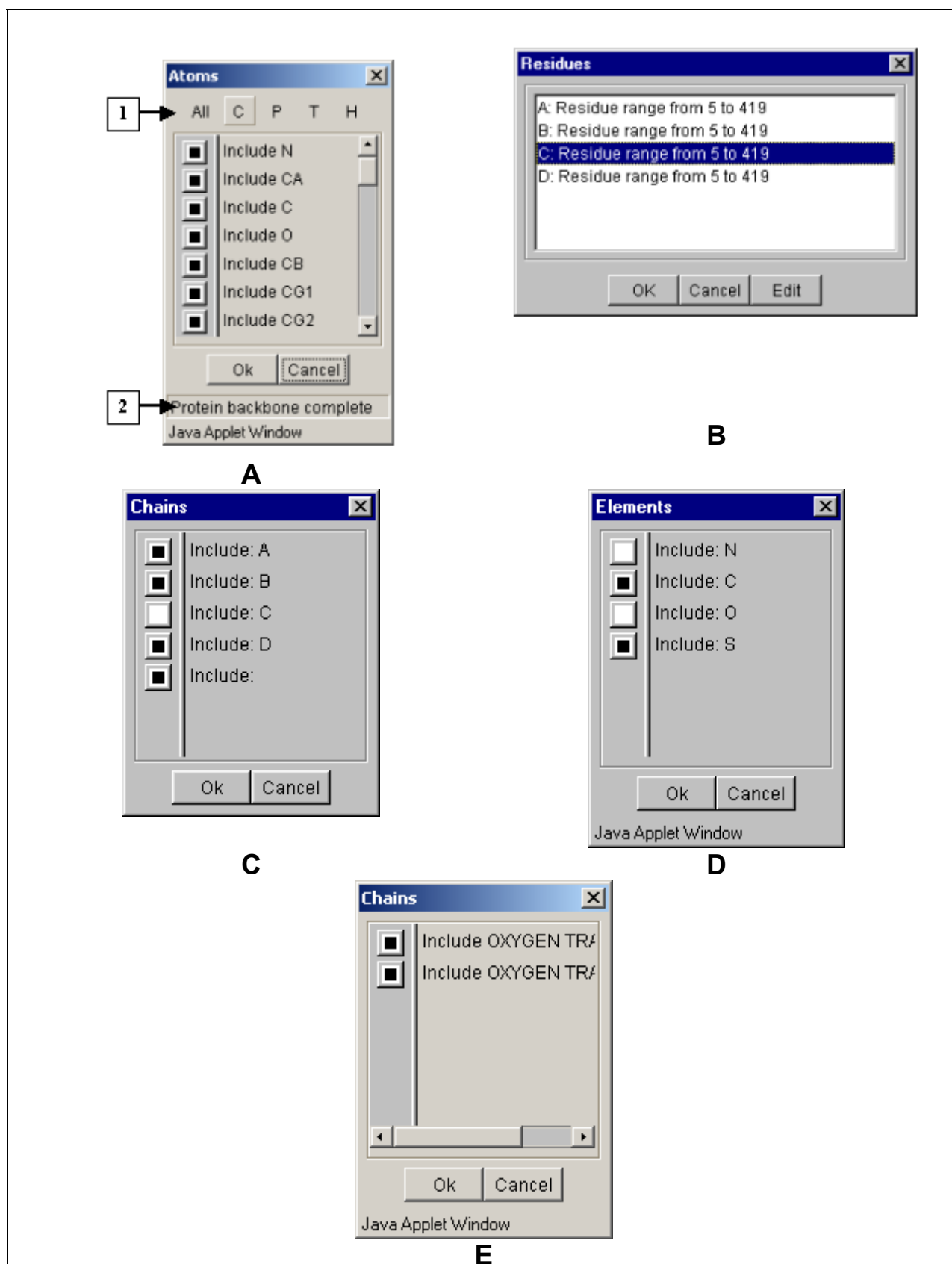


Figure 3.5.2.

A. Atoms dialog window. **B. Residues** dialog window. **C. Chains** dialog window. **D. Elements** dialog window. **E. Models** dialog window.

1. Control panel buttons. 2. Status Bar.

The **Residues** dialog window (3.5.2. B) contains the list of chains' names with ranges of displayed residues for each chain. To change a range, select the name of a chain with appropriate range and then press **Edit** button. A dialog window with the title containing the chain's name (e.g. **Chain: A**) will appear. In this window, the range of displayed residues can be defined (fig.3.5.3). To change a range, enter the required values into **From** and **To** fields. As soon as **Set** button on **Min** bar is pressed, the number of the first chain residue is to be entered. Similarly, as soon as **Set** button on **Max** bar is pressed, the last chain residue is to be entered.

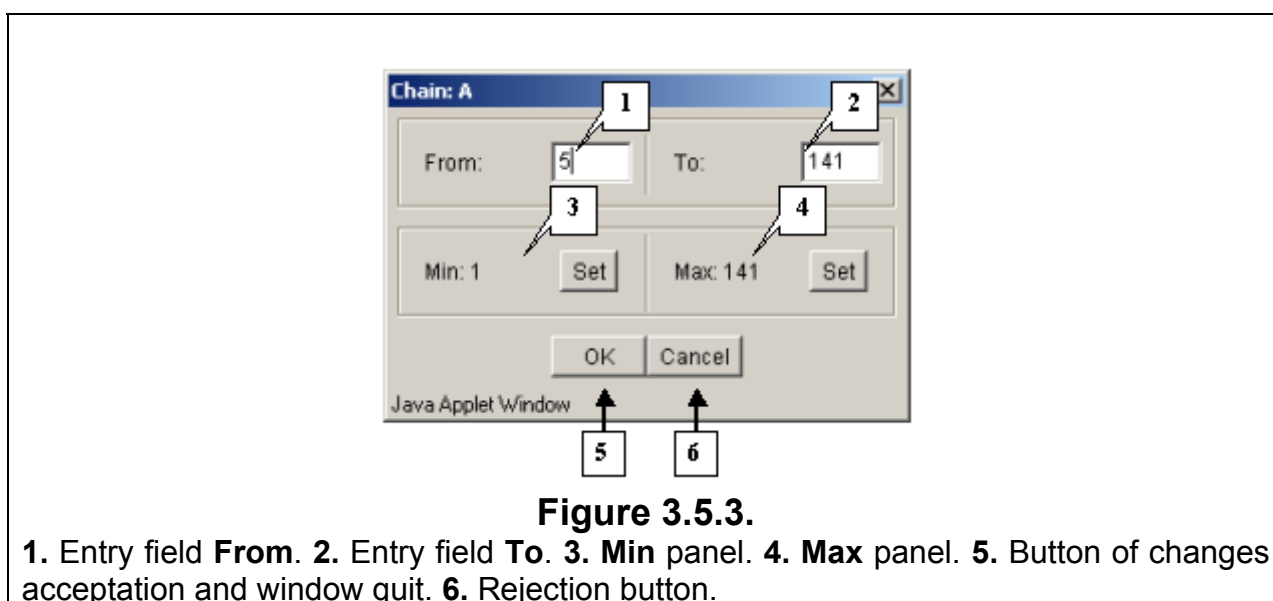


Figure 3.5.3.


1. Entry field **From**. 2. Entry field **To**. 3. **Min** panel. 4. **Max** panel. 5. Button of changes acceptance and window quit. 6. Rejection button.

Model options dialog window control buttons:

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

3.6. Options dialog window

On the **Options** dialog window (Fig. 3.6.1), 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  toolbar button.

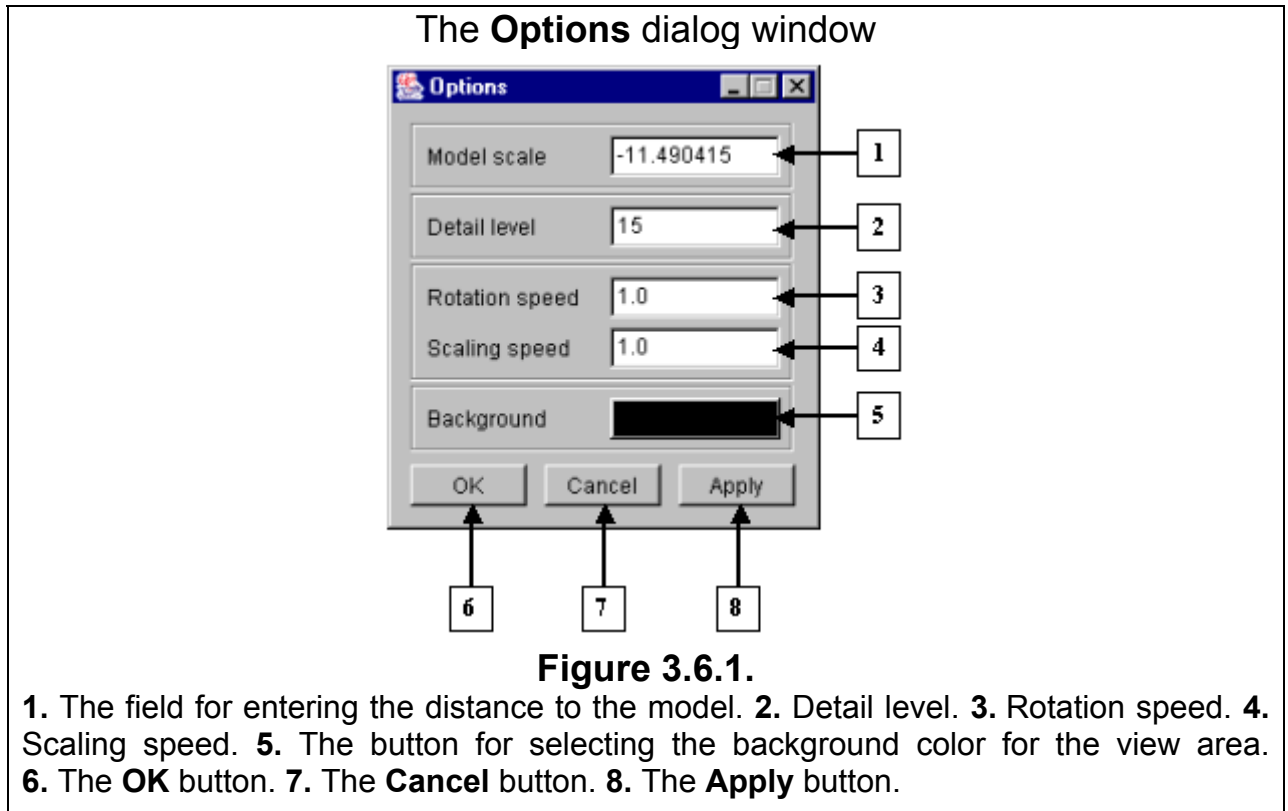
In the **Options** dialog window, you can change:

- 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 3.7 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.
- Click **Apply** to accept changes without quit the window.



3.7. Color dialog

The **Color dialog** window (fig. 3.7.1) provides the color selection. Color can be selected by several means:

- Using the basic colors set. It requires the clicking on the square with desired color. The selected color will appear on the new color preview bar. To accept the choice press the **OK** or **Apply** buttons.
- Using the customized colors set. It requires the clicking on the square with desired color of this set. The selected color will appear on the new color preview bar. To accept the choice press the **OK** or **Apply** buttons. It's allowed to change the set of colors. It requires the clicking on a square of this set. Using slider and switches of HSB and RGB models fields select a desired color. Upon the **Set Custom Color** button is pressed the selected color will appear in a selected square of the set and on the new color preview bar.
- Using the new color selection. For this purpose use the slider and switches of HSB and RGB color models fields. The selected color will appear on the new color preview bar. To accept the choice press the **OK** or **Apply** buttons.

If it's required to be back to old color click the mouse on the previous color preview bar and press the **OK** or **Apply** buttons.

Comment. The **OK** button provides the acceptance of changes made and quit the window. The **Cancel** button provides the rejection of changes made and quit the

window. The **Apply color** button provides the acceptance of changes made without quit the window.

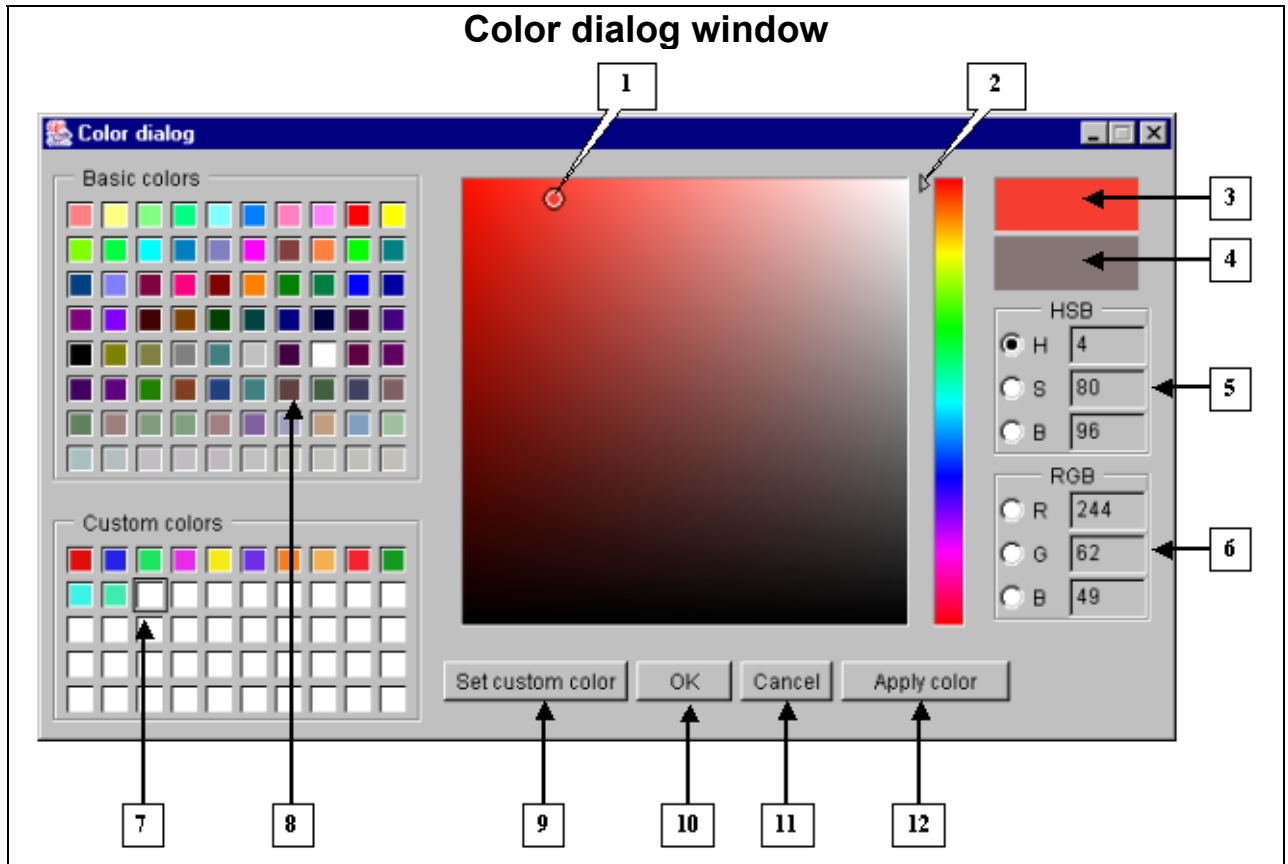


Figure 3.7.1.

1. Color selection area. 2. Slider. 3. New color preview bar. 4. Previous color preview bar. 5. HSB color model. 6. RGB color model. 7. Customized colors. 8. Basic colors set. 9. Button for color customizing. 10. Button of color acceptance and quit the window. 11. Button of choice rejection and quit the window. 12. Button of color acceptance without quit the window.

3.8. *Matrix* dialog window

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

- Select the **Window>Matrix dialog** 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.

In the Model identifiers drop-and-down list, select the identifier of the model to be displayed as a matrix (Fig. 3.8.1). The list contains identifiers of all loaded models.

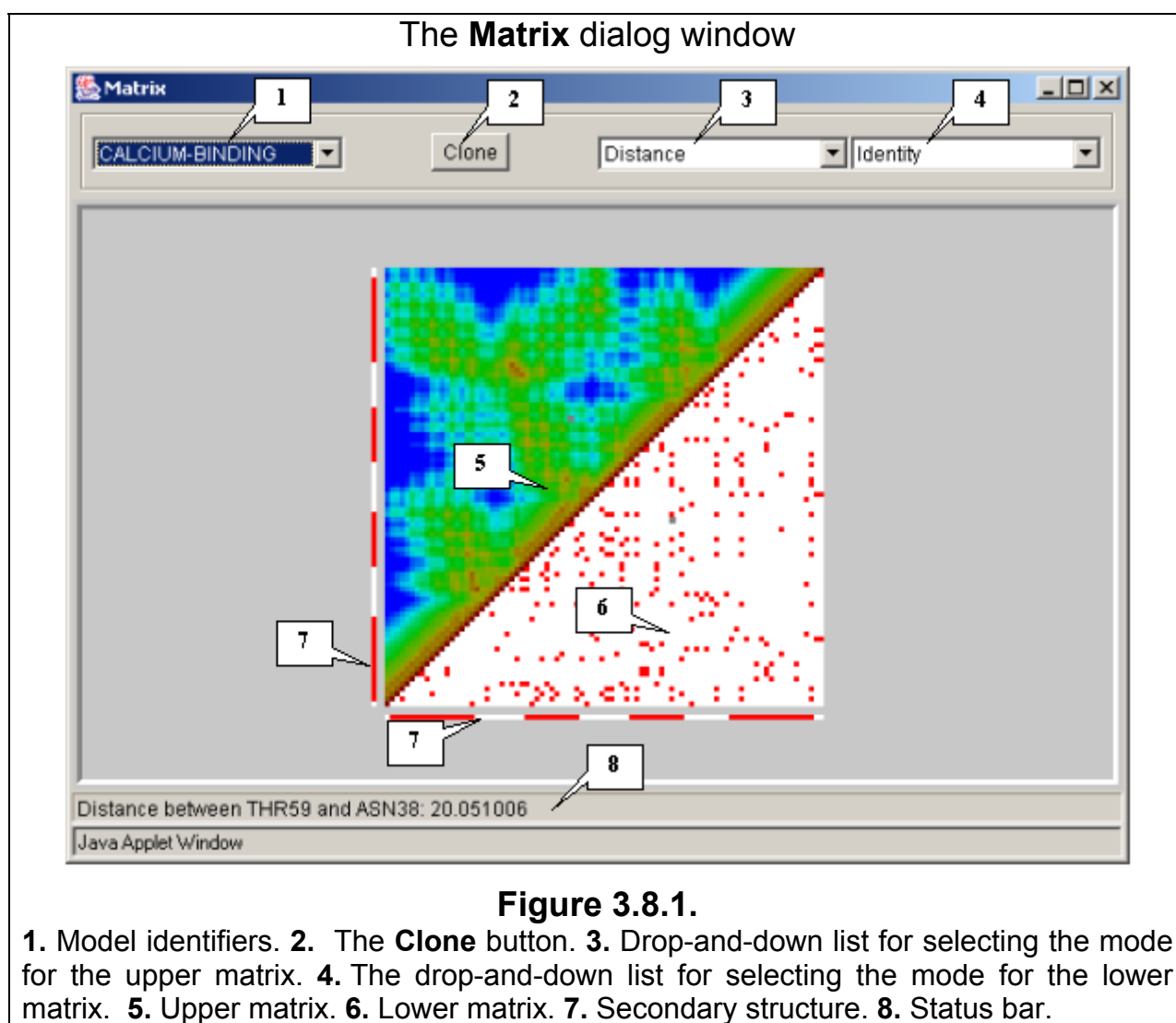
The upper matrix mode can be selected in the drop-and-down list for the upper matrix and the lower matrix mode can be selected in the drop-and-down list for the lower matrix (Fig. 3.8.1). The following matrix modes are available:

- **Distance** – Show distances between matrix elements.
- **Identity** – Show similarities between the types of elements.

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.

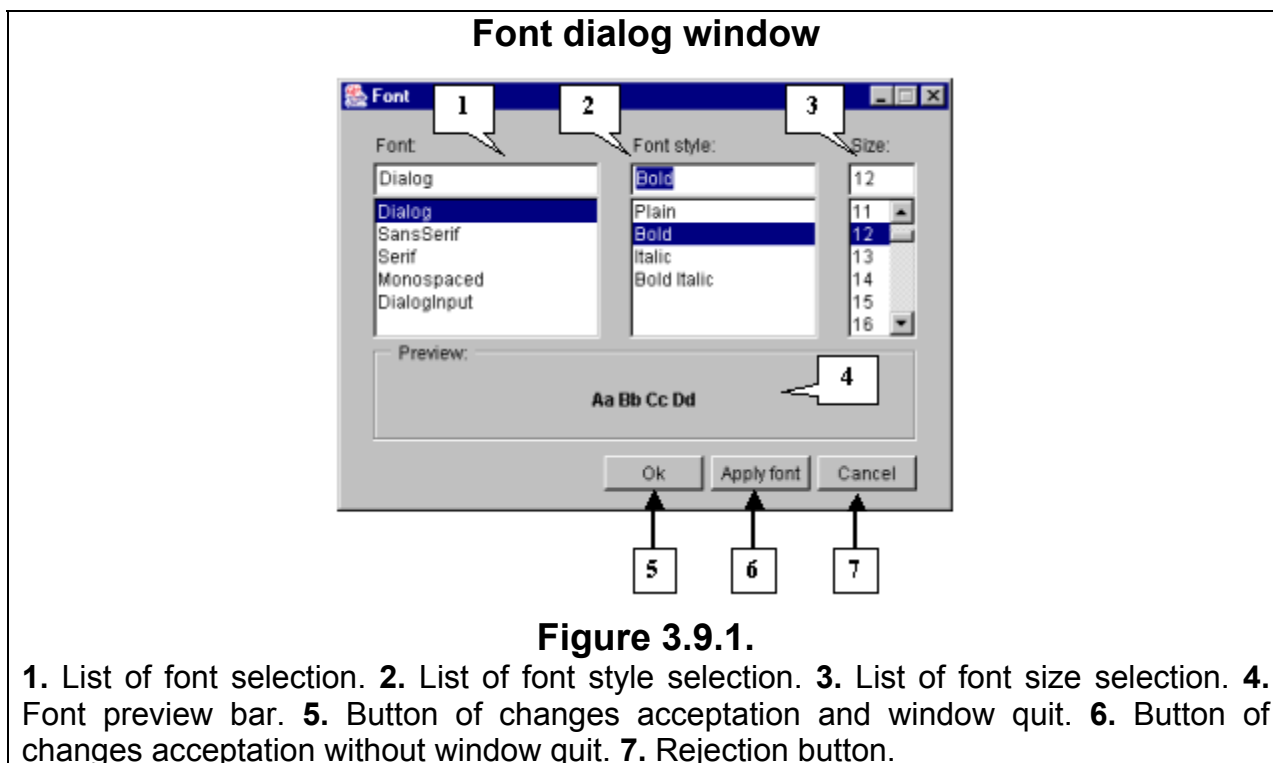
Click the **Clone** button to make a copy of this dialog window.



3.9. Font dialog window

The **Font** dialog window (fig. 3.9.1) provides the setting of font parameters.

- The **Font** list provides the selection of a desired font.
- The **Font style** list provides the selection of the font style.
- The **Size** list provides the selection of the font size.
- The **Preview** bar provides the preview of selected font.
- The **OK** button provides the acceptance of changes made and quit the window.
- The **Apply font** button provides the acceptance of changes made without quitting the window.
- The **Cancel** button provides the rejection of changes made and quit the window.



4. References

1. [www.rcsb.org/pdb/info.html#File Formats and Standards](http://www.rcsb.org/pdb/info.html#File_Formats_and_Standards)