Molecular Dynamics Visualisation (MDV) User Guide

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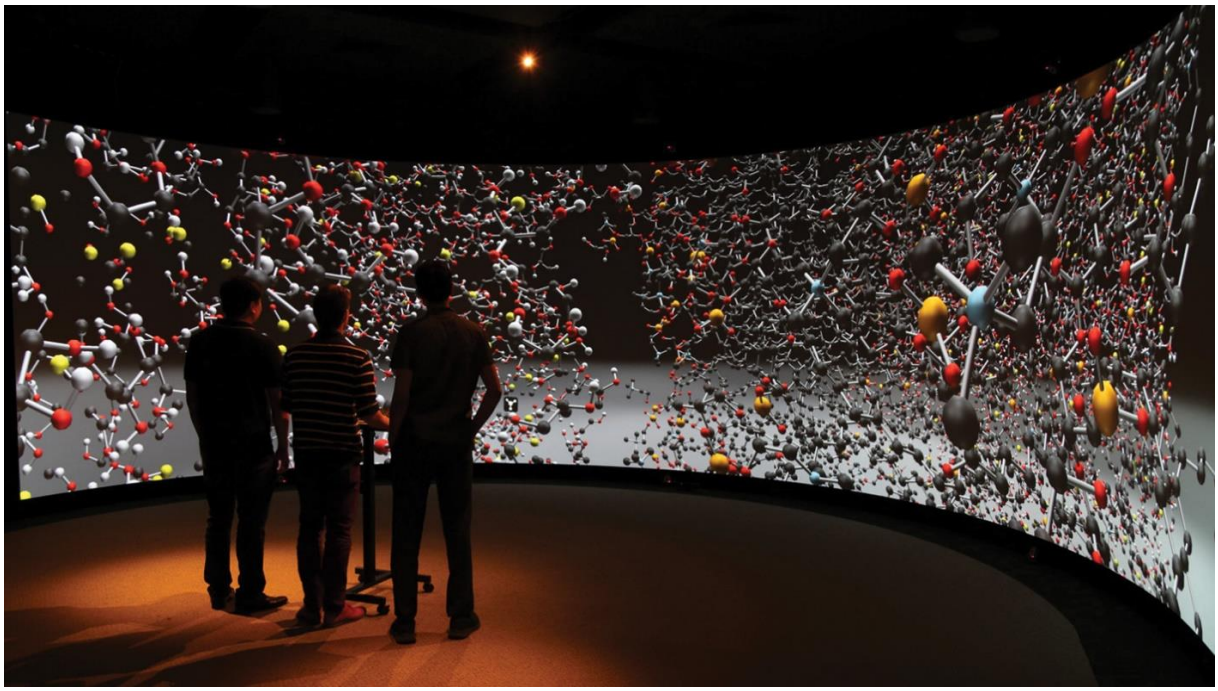
Overview

Molecular Dynamics Visualization (MDV) is a tool developed by Curtin University to display molecular dynamics simulations on a large-scale stereo cylindrical display at Curtin HIVE.



Features

- Load and rendering of molecular topology files. Includes rendering support for protein secondary structures. Supports PDB, Gromacs and XYZ formats.
- Load of molecular trajectory files and rendering of primary and secondary structure animation of the trajectory. Supports XTC and DCD formats.
- Stereo capable user interface built in world space with a mouse pointer in 3D space.
- Detailed visualisation options with support for modifying molecular representation at both a protein residue and an atom by atom level.

- Ability to save and load visualisation settings for molecular structures.
- Load multiple molecules into the same 3D visual space and translate and rotate molecules in relation to each other.
- Realtime calculation and visualisation of VDW energies and electrostatic forces between pairs of moving molecules.

View and Molecule Control

View Control

The camera (view on the molecules) can be moved with the keyboard and mouse, or a space mouse. Space Mouse support must be enabled in the ‘Other’ settings panel in the user interface.

Keyboard and Mouse controls

Hold the right mouse button down and move the mouse to rotate the camera.

Hold the right mouse button down and press a movement key to move the camera.

W, A, S, D keys – forward, left, backward and right

Q, E keys – down and up

Space Mouse controls

Move the space mouse in the direction you want the camera to move.

Twist the space mouse to rotate the camera on the vertical axis. Only yaw rotation is supported on the space mouse, pitch and roll are disabled.

Molecule Control

Similar to camera movement, molecules can be moved with the keyboard and mouse, or a space mouse.

A molecule must be selected in the ‘Molecules’ settings panel in the user interface to enable control of that molecule. You can also press the TAB key to cycle through the currently loaded molecules. Only one molecule can be moved at a time.

Keyboard and Mouse controls

Hold the shift key and move the mouse to move the molecule up, down, left and right

Hold the shift key and ctrl key and move the mouse to move the molecule forward, backward, left and right

Hold the ctrl key and move the mouse to rotate the molecule toward, away, left and right of camera.

Hold the alt key and move the mouse to rotate the molecule on the vertical axis

Space Mouse controls

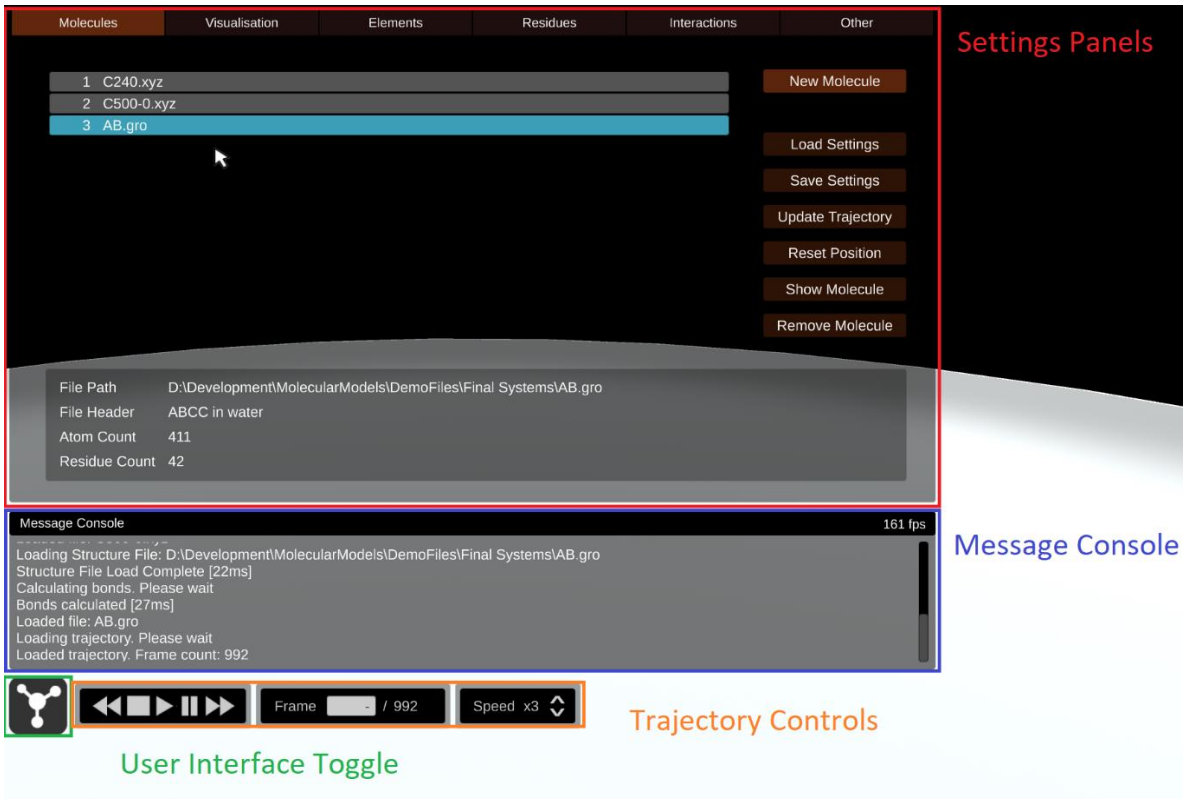
Hold down the shift key and move the space mouse to move the molecule.

Hold down the ctrl key and rotate the space mouse to rotate molecule.

User Interface

Apart from camera and molecule position and rotation, all application control is done through the user interface.

The user interface contains four main areas. These are the toggle button, settings panels, message console and the trajectory controls.



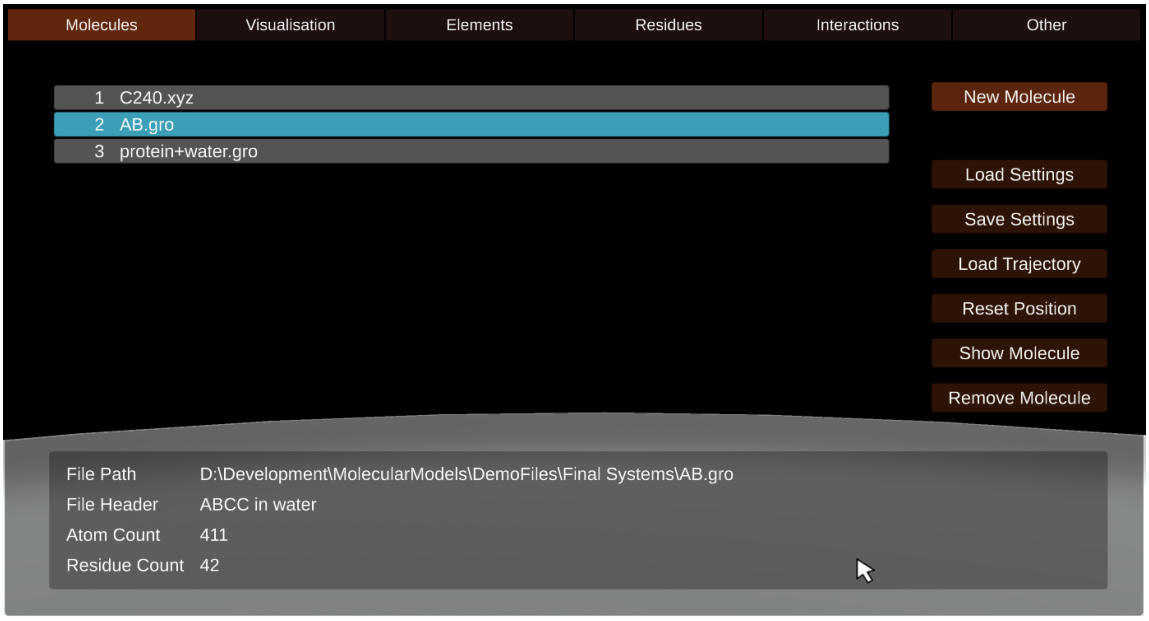
Toggle Button

The toggle button is always visible. It can be clicked on with the mouse cursor to show and hide the settings panels and message console. The toggle button doesn't hide the trajectory controls (if they are showing), this allows control of a trajectory animation while the UI is hidden. The user interface can also be toggled with the escape or tilde key.

Settings Panels

The settings panels are the main interface for loading molecules and manipulating their visual representation. The settings panels are a series of screens that are available one at a time by clicking on the buttons at the top of the panels.

Molecule Settings



The molecule settings panel allows the user to load molecule data from structure and trajectory files, load and save molecule visualisation settings and to select molecules for manipulation in other settings panels or via movement controls.

Once a molecule is loaded from a molecule structure file it appears in the list on the top left of the panel. There is no limit on the number of molecules that can be loaded but note that loading a large number of molecules can reduce application performance.

When a molecule is loaded it is positioned according to the coordinates in the input file and the camera centred on the molecule. This could lead to the molecule and

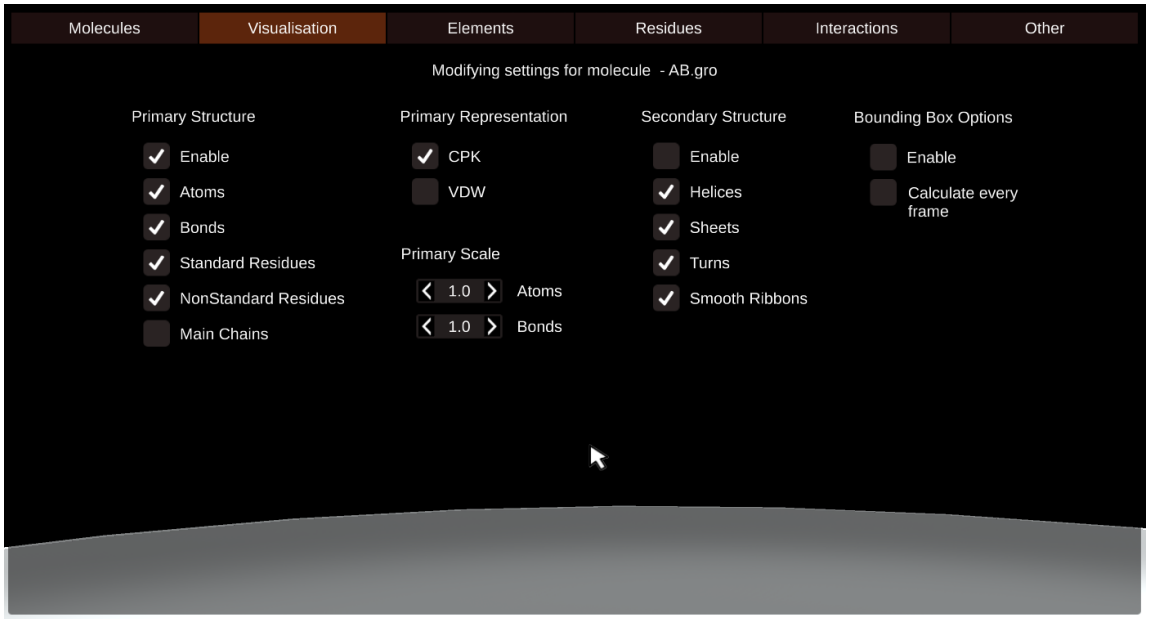
view being under the ground if the ground is currently visible (see ’Other’ settings panel)

Molecules in the molecule list can be selected to perform actions. You can do this by clicking on the molecule in the list with the left mouse button. The currently selected molecule is highlighted in blue and its details are displayed in the information section at the bottom of the panel. You can also press the TAB key to iterate through the list of molecules in the molecule panel. This works regardless of whether the panel is showing or not.

All of the buttons on the right-hand side of the panel perform actions on the selected molecule. The ‘Visualisation’, ‘Elements’ and ‘Residues’ panel also perform actions on the currently selected molecule.

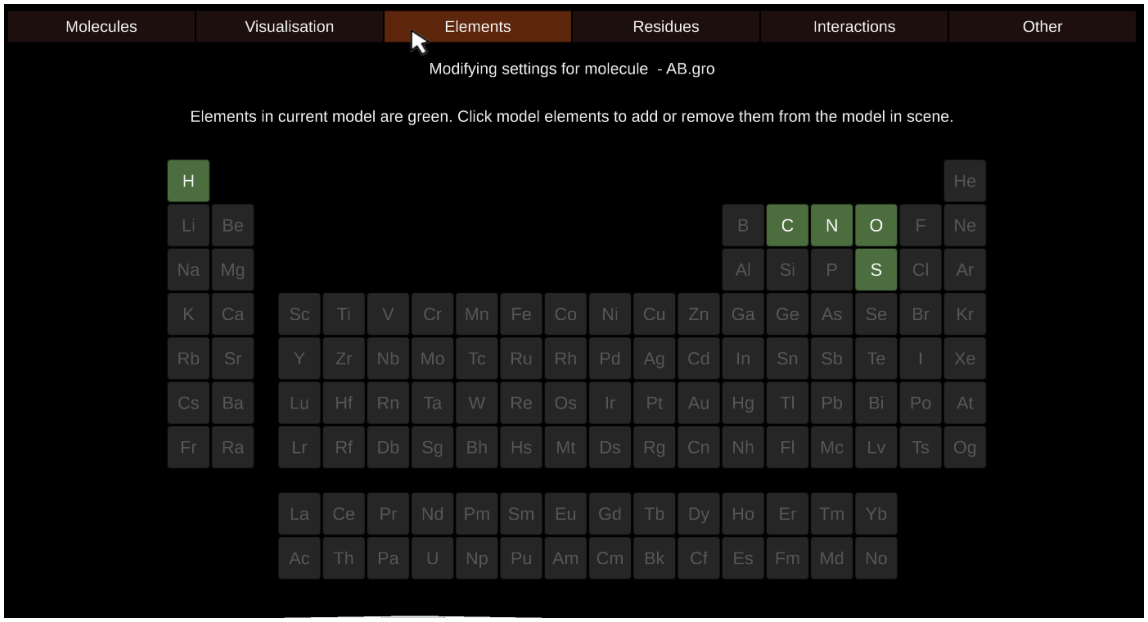
The load and save settings buttons allow the user to save and reload the visualisation settings for currently selected molecule. The visualisation settings include all settings from the ‘Visualisation’, ‘Elements’ and ‘Residues’ panels. When you save a settings file, it will also save the current path to the molecule structure, the path to any loaded trajectory and the current camera and molecule positions. Settings files can be loaded using the ‘New Molecule’ button where the molecule will be loaded along with the settings. If you use the ‘Load Settings’ button the settings in the settings file will just override the visualisation settings on the currently selected molecule.

Visualisation Settings



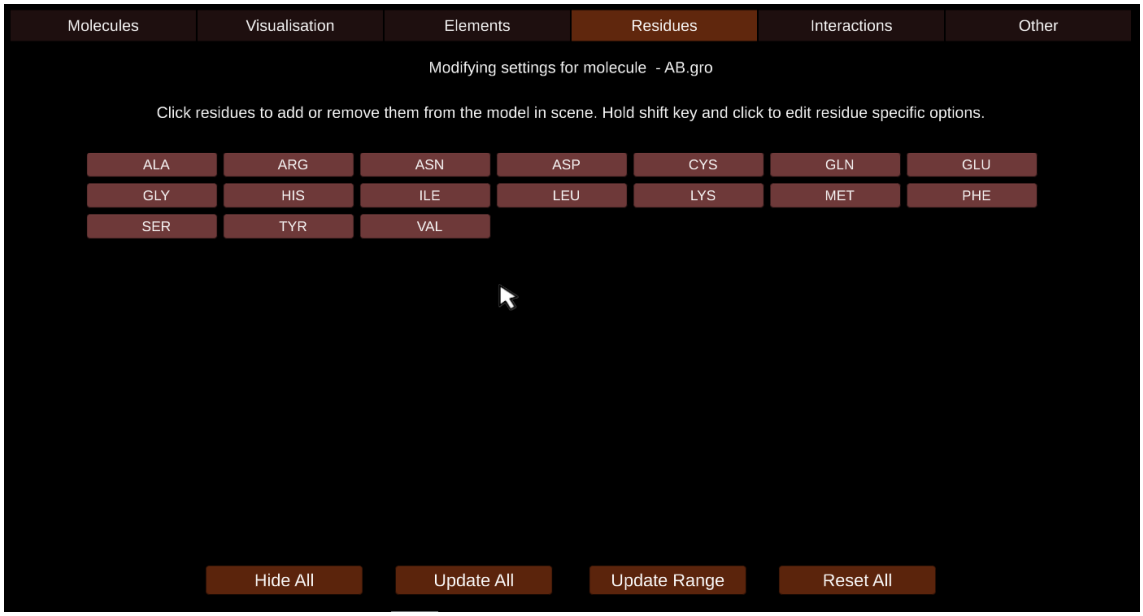
The visualisation settings panel allows the user to modify general visualisation settings for the currently selected molecule (molecule name show at top of panel). You can use the TAB key to rotate through the loaded molecules while on this panel.

Element Settings



The element settings panel allows the user to modify the displayed elements for the currently selected molecule (molecule name show at top of panel). You can use the TAB key to rotate through the loaded molecules while on this panel.

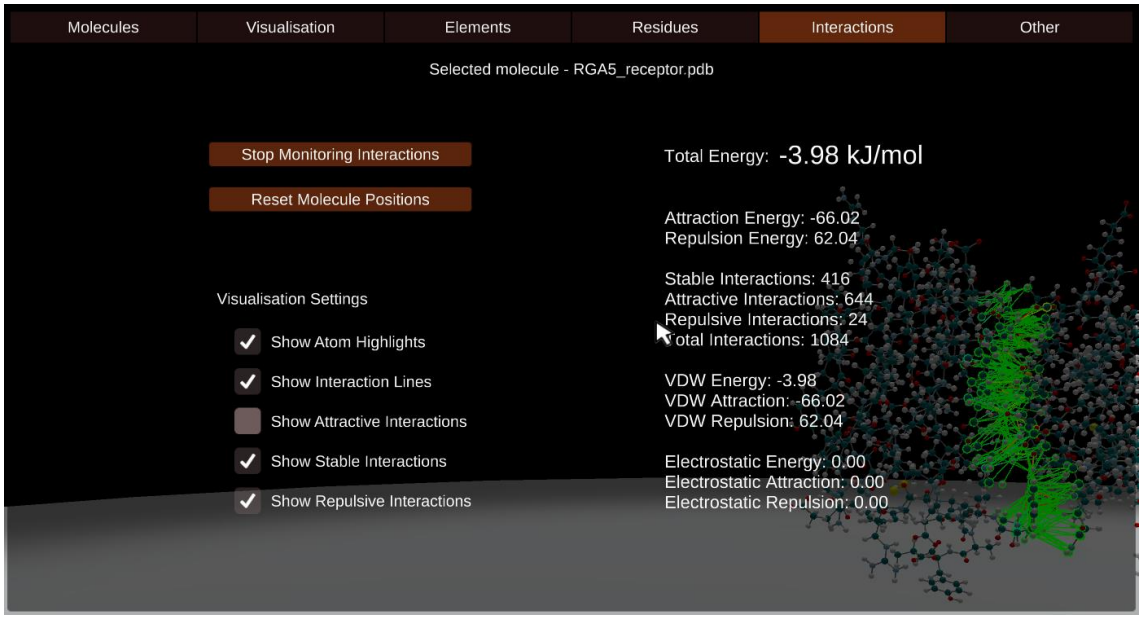
Residue Settings



The residue settings panel allows the user to modify the visualisation of the residues in the currently selected molecule (molecule name show at top of panel). You can use the TAB key to rotate through the loaded molecules while on this panel.

Residues will only display if the molecule input file has residue information.

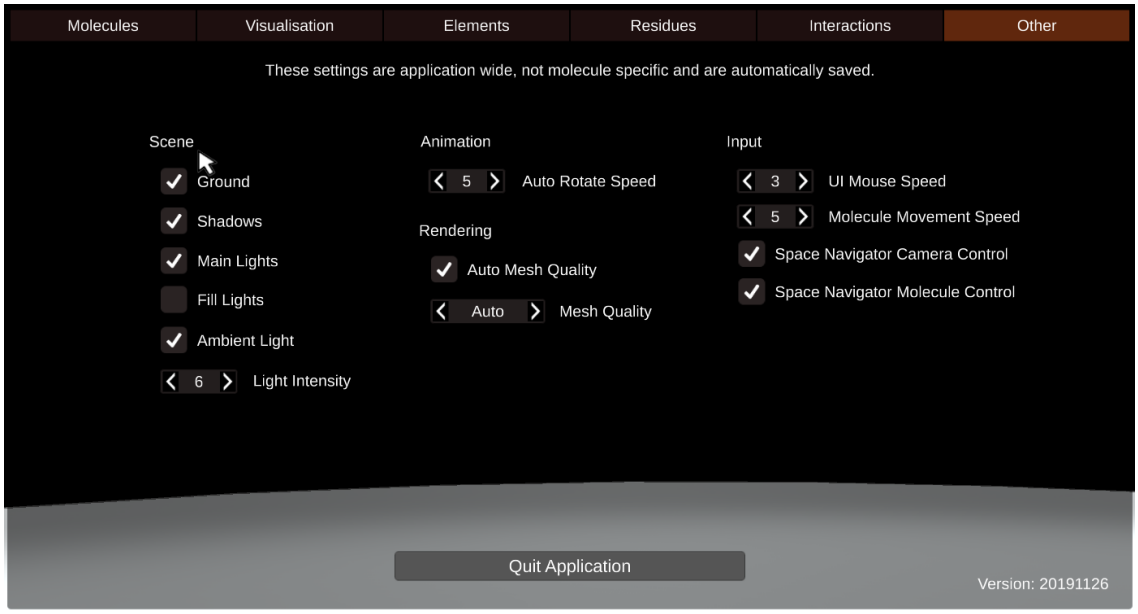
Interaction Settings



The interaction settings panel allows the user to enable the calculation and visualisation of intermolecular forces between two molecules. Calculations can only be enabled when exactly two molecules are loaded. If a molecule if added or removed while calculations are active then the calculations will be stop. You can use the ‘Reset Molecule Positions’ to move the molecules to the positions they were in when they were first loaded. This works the same as the ‘Reset Position’ button on the ’Molecules’ settings panel but on both molecules at the same time.

Settings on the interaction settings panel are not saved and reset every time the application is restarted.

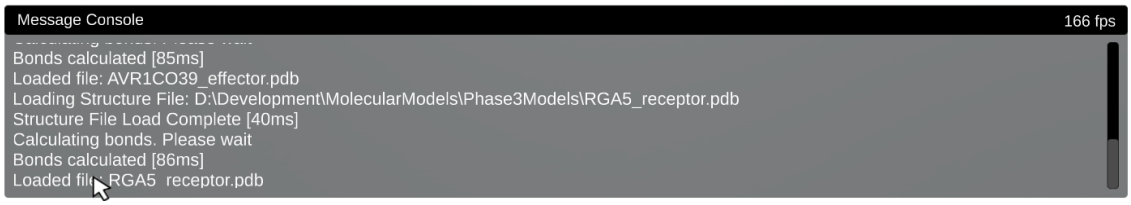
Other Settings



The other settings panel allows the user to modify general settings that are not molecule specific. The settings on this panel are automatically saved to the local system and will persist between application uses.

The Auto Mesh Quality toggle will enable the application to determine the mesh quality of the atom and bonds in the visualisation. With this enabled the application will adjust the render quality on molecules as molecules are added or removed from the scene.

Message Console



The message console show messages to the user responding to actions taken in the user interface. It displays file load and save progress, error messages and other important information.

Trajectory Controls

The trajectory controls will only show when a trajectory is loaded and the molecule with the trajectory is currently selected in the user interface.

The controls can be used to manipulate the display of the trajectory animation. The frame number can be altered directly by selecting the frame number box and entering a number.