## Mouse Controls

### Selection

| Action | Result |
|---|---|
| **Click on:** | |
| Atom | Selects atom |
| Residue | Selects residue |
| Annotation lane (H) | Activate annotation coloring & linking |
| Feature (H) | Selects feature |
| Element in sequence overview (I) | Selects secondary structure element |
| Background | Clears selection |
| **Ctrl + click on:** | |
| Selected object | Extends selection to next level in hierarchy |
| Unselected object | Adds object to selection |
| **Ctrl + Shift + click on:** | |
| Selected object | Removes object from selection |
| Deselected object | Removes next level of hierarchy from selection |
| **Shift + click** | Selects a range of residues |
| **Alt + click** | Selects whole chain |

### Rotation and Translation

| Action | Result |
|---|---|
| Drag | Rotates structure around X & Y axes |
| Ctrl + drag (left & right) | Rotates structure around Z axis |
| Right button drag | Translates structure along X & Y axes |

### Zooming

| Action | Result |
|---|---|
| Shift + drag (up & down) | Zooms out & in |
| Double click | Auto zooms to object |
| Shift + double click | Auto zooms to residue range or ligand |
| Alt + double click | Auto zooms to whole chain |

## Keyboard Controls

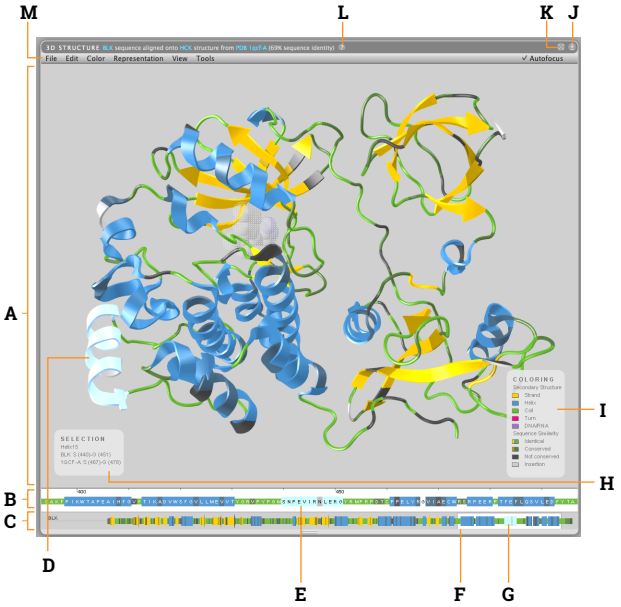
| Action | Result |
|---|---|
| A-Z or * | Finds text patterns in sequences |
| Esc | Clears selection |
| Enter | Auto zooms to selection; if no selection is made, zooms to whole structure |
| Shift + Enter | Auto zooms to whole structure |
| Right arrow | Selects next residue in sequence |
| Left arrow | Selects previous residue in sequence |
| Shift + right arrow | Adds next residue to selection |
| Shift + left arrow | Adds previous residue to selection |
| Up arrow | Selects next highest level in hierarchy |
| Tab | Selects next object, depending on selected object |
| Shift + Tab | Selects previous object |
| 2 | Rotates about X axis (anticlockwise) |
| 8 | Rotates about X axis (clockwise) |
| 4 | Rotates about Y axis (clockwise) |
| 6 | Rotates about Y axis (anticlockwise) |
| Ctrl + 2, 4, 6 or 8 | Rotates in 45° steps (axes as above) |
| Alt + 2, 4, 6 or 8 | Translates (axes as above) |
| + | Zooms in stepwise |
| - | Zooms out stepwise |
| Ctrl + C | Copies selection to paste buffer |
| Ctrl + V | Pastes a text string from another program into the search buffer |
| Ctrl + L | Selects all ligands |
| Ctrl + R | Resets view to initial state |
| Ctrl + S | Saves view state |
| Ctrl + Shift + L | Labels selection (toggle) |
| Ctrl + Shift + W | Toggles wireframe representation |
| Alt + Ctrl + PrtSc | Prints screen image to paste buffer |

Aquaria 3D Viewer is based on SRS 3D Viewer, originally developed at LION bioscience AG.

# AQUARIA 3D VIEWER

# Quick Reference Card

version 1.0




**A** Structure view: displays 3D structure

**B** Sequence details view: click to select a residue

**C** Sequence overview: shows all sequences in the structure

**D** Highlight: indicates selected region of structure

**E** Highlight: indicates selected residues

**F** Focus box: indicates the region shown in sequence details view; drag to change the focus

**G** Highlight: indicates selected region of the sequence

**H** Selection overlay: text description of current selection

**I** Legend for current coloring scheme

**J** Click to launch stand-alone application

**K** Click to expand 3D view to full window

**L** Click to see explanation of 3D view

**M** Applet menu

# Applet Menu

## File

| Menu option | | Effect |
|---|---|---|
| Save | ⌥⌘S | Saves view state (automatically used when structure is next loaded) |
| Reload | | Reloads saved view state |
| Revert | ⌘R | Reverts the entire view (rotation, representation, coloring etc.) to the initial state. |
| Export Image... | | Save the current view as a PNG image. You can specify image dimensions and background color (white/grey/black). |
| Print... | | Opens the current view in a separate window for printing. You can specify image dimensions, background color, and toggle color legend and selection overlays. |

## Edit

| Menu option | | Effect |
|---|---|---|
| Copy | ⌘C | Copies residues in ClustalW format, for pasting into text processor (e.g. Notepad) |
| Paste | ⌘V | Pastes text string from another program; finds occurrences of string in all sequences |
| Select All | ⌘A | Selects all objects |
| Select Ligands | ⌘L | Selects all ligands |
| Select Proximity | ⇧⌘P | Selects everything within 4Å of current selection |
| Select Water | | Selects all water molecules in the structure |

## Color

| Menu option | Effect |
|---|---|
| Sequence Similarity | Colors selection by sequence similarity (default) |
| Secondary Structure | Colors selection by secondary structure |
| Molecule | Colors selection by molecule type |
| Chains | Colors selection by chain |
| Hydrophobicity | Colors selection by hydrophobicity index |
| Polarity | Colors selection by charge type |
| Temperature | Colors selection by B-factor (high B-factor is correlated with high temperature) |
| Element | Colors selected atoms by chemical element type (CPK standard). |
| Choose Color... | Opens a color picker to apply chosen color to the selection |

## Representation

| Menu option | | Effect |
|---|---|---|
| Visible | ⇧⌘V | Displays / hides selection |
| Transparent | | Makes selection slightly transparent |
| Ribbon | ⇧⌘R | Cartoon representation of the backbone |
| C-alpha Trace | ⇧⌘T | Straight lines connecting all Cα atoms |
| Wireframe | ⇧⌘W | Atoms connected by straight lines |
| Spacefill | ⇧⌘F | Atoms as spheres with van der Waals radii |
| Ball&Stick | ⇧⌘B | Atoms as spheres, bonds as sticks |
| Surface | | Calculates the molecular surface of the selection |
| Remove All Surfaces | | Removes any calculated surfaces |

## View

| Menu option | | Effect |
|---|---|---|
| Normal | | Proteins & DNA/RNA shown as ribbons, ligands as spacefill, disulfide bonds as ball & stick. Uses Sequence Similarity coloring scheme. |
| Ligand Binding Sites | | Highlights ligand & binding site interactions. Polypeptide chains shown as Cα trace. All atoms within 4Å of ligand shown as wireframe. |
| Spin | space | Toggles spinning around Y axis on & off (drag to change spin axis) |
| Zoom to Selection | ⏎ | Auto zooms to current selection |
| Zoom Out | ⇧⏎ | Auto zooms to whole structure |
| Show PDB Sequence | | Displays sequence track for current structure |
| Show Water | | Displays all water molecules in the structure |
| Mouse Controls | | Toggles mouse controls overlay on & off |
| Color Legend | | Toggles color legend on & off |
| Selection | | Toggles selection overlay on & off |

## Tools

| Menu option | Effect |
|---|---|
| **Features** | |
| > Create New... | bases new annotation on current selection |
| **Label** | |
| > Molecules | Labels each molecule |
| > Chains | Labels each chain |
| > Secondary Structure | Labels each secondary structure element in selection |
| **Calculate** | |
| > Distance | Calculates the closest interatomic distance between two selected regions |
| > Atomic Contacts | Calculates van der Waals overlaps between selection & rest of structure |
| > Remove All Distances | Removes any displayed distances |
| > Hydrogen Bonds | Calculates hydrogen bonds for current selection |
| **Advanced Settings** | |
| > Move as C-alpha Trace | Enables fast rotation and translation |
| > High Quality | Display smooth curves with specular highlights and shading |
| > About | Display build information & authors |