4.4 Moving molecules independently with the mouse:

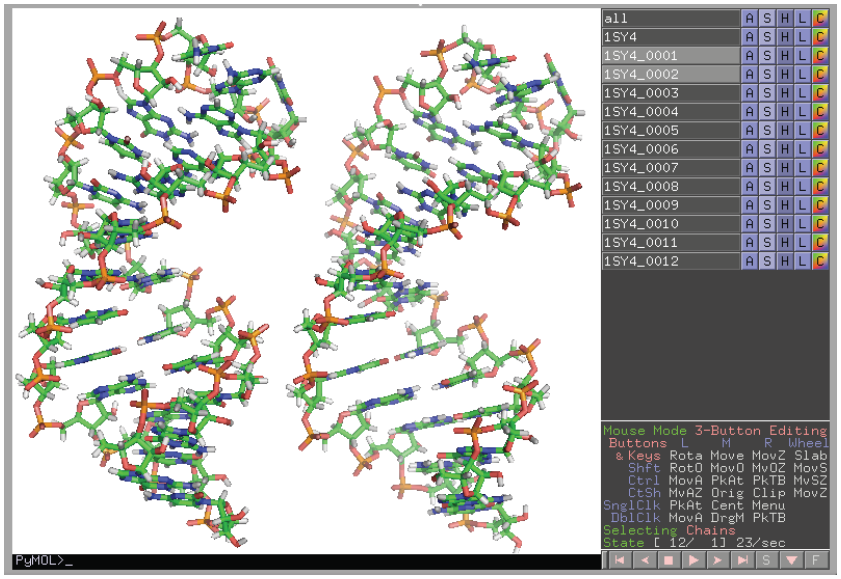
It is possible to move molecules relative to each other by using the mouse in editing mode. This is a brief exercise to try this:

✔ TASK

√ - **Click** on the word "**all**" within the names panel: all images will disappear from view
√ - **Click** on the **2** individual **objects** e.g. 1SY4_0001 and 1SY4_0002 to bring them to full view
√ - **Change** to the mouse editing mode with the menu:
Mouse > 3 Button Editing Mode

√ - **Hold** the **SHIFT** key **and click** on any one of the 2 structures with the **middle button**. This will allow you to move the structure to the right or left (translation).

√ - Now **move the 2 structures apart.**

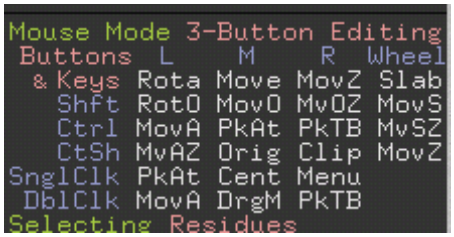


Note: in this mode the left button still rotates and the right button still moves on the Z axis. Holding the SHIFT key restrict the movement to the clicked molecule.

✔ INFO- Summary of the mouse method:

- **Switch to 3-botton mouse editing** with the Mouse menu.

The table at bottom right summarizes the possible movements. The mouse movement ending with "O" are related to object rotations: Shift+Left button = RotO (rotate object). Shift+Middle button= MovO (move object), Shift+ Right button=MvOZ (translate the object



along the Z axis).

- **Click on the object** (molecule) you want to rotate or translate.
- **Apply the proper mouse/keystroke combination** for rotation, translation, or moving along Z (toward or away from you)

✔ **TASK: Quit or Reinitialize PyMol (File menu)**

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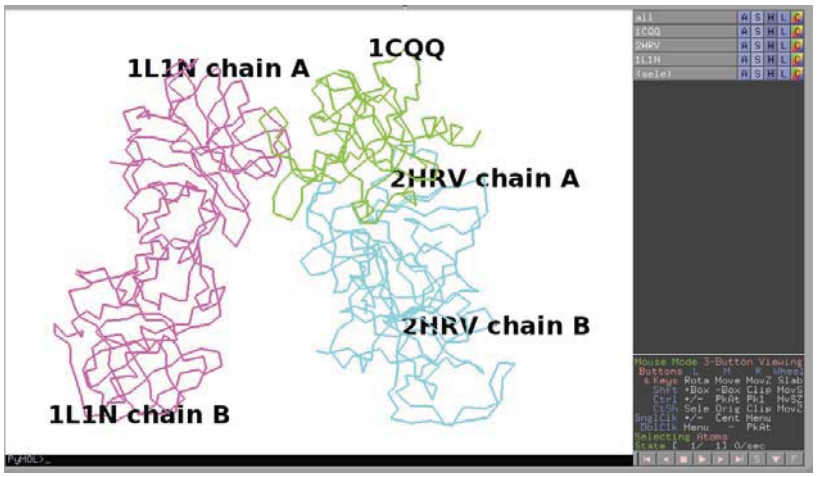
5 *PyMol - Exercise R*: Automatic Structures Superimposition

✔ **TASK**

Preliminary:

√ - **Open** a web **browser** to the PDB site http://www.rcsb.org/pdb/
√ - search and **retrieve 1CQQ**, **2HRV**, **1L1N**
√ - **Open** a **new PyMol** (MacPyMol) **session**
√ - **load** the **3 PDB files** saved (**load** command or **File > Open** menu) in the order:1CQQ.pdb , 2HRV.pdb, 1L1N.pdb
√ - Change **background** to **white** (Display menu)
√ - Hide everything and show ribbons: (Names Panel)

all > H > everything
all > S > ribbon



set label_color, black

set label_size, 32

set label_font_id, 7

√ **- Change** the mouse selection mode to chain: **Mouse > Selection Mode > Chains**
√ **-** Using the above image as a guide, **click** on **2HRV chain B.** This

places the B chain within the selection (sele) name.
√ **- Extract** the selection to an object: **(sele) > A > extract object**
√ **- Rename** the object : **obj1 > A > rename object** and **type 2HRV_B** when asked
√ **- Repeat** the process with **1L1N chain B:**
Click on chain B
(sele) > A > extract object
obj02 > A > rename object
type 1L1N_B
√ **-** We are now ready to attempt superimposition.

5.1 Automatic superimposition with Action menu

INFO

```
PDB ID  TITLE
1CQQ    TYPE 2 RHINOVIRUS 3C PROTEASE WITH AG7088 INHIBITOR
2HRV    2A CYSTEINE PROTEINASE FROM HUMAN RHINOVIRUS 2
1L1N    POLIOVIRUS 3C PROTEINASE
```

TASK

To align all of the objects to 1CQQ, use the following menu cascade:

1CQQ > A > align > all to this