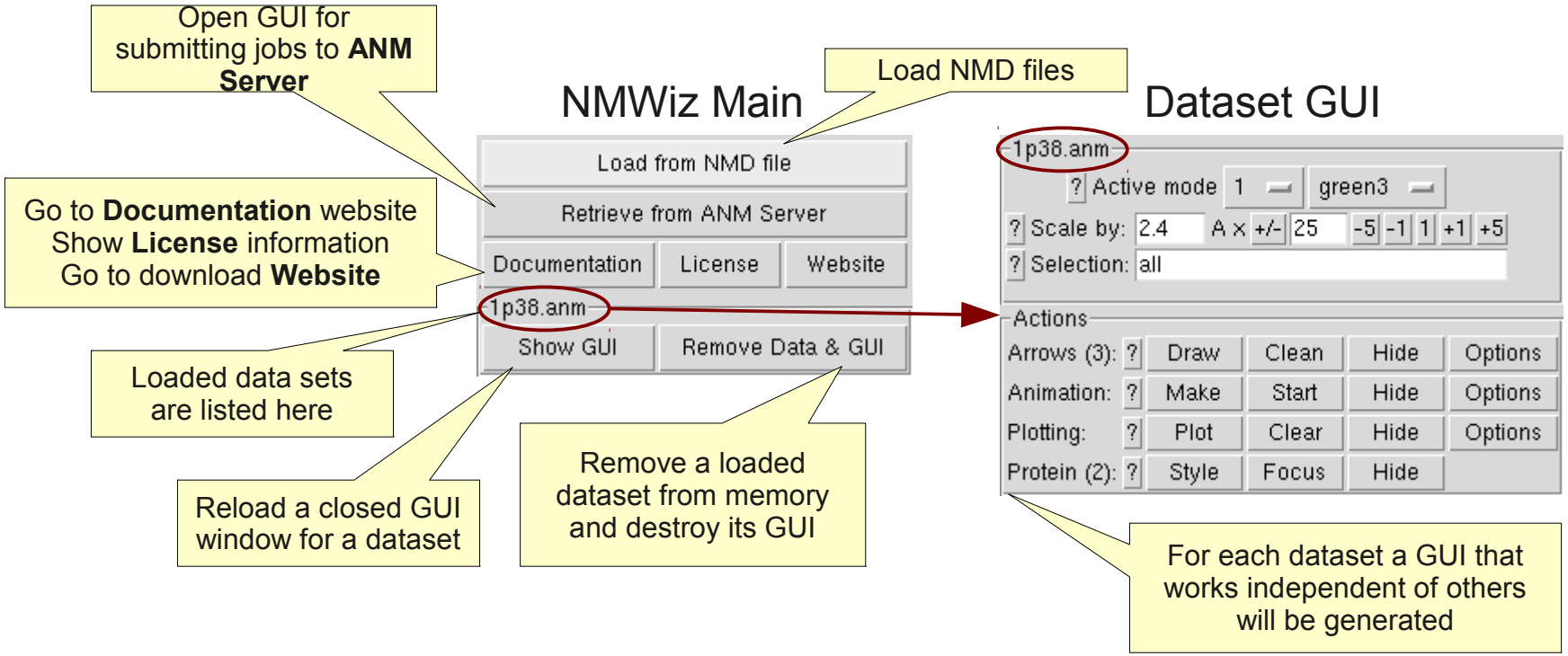
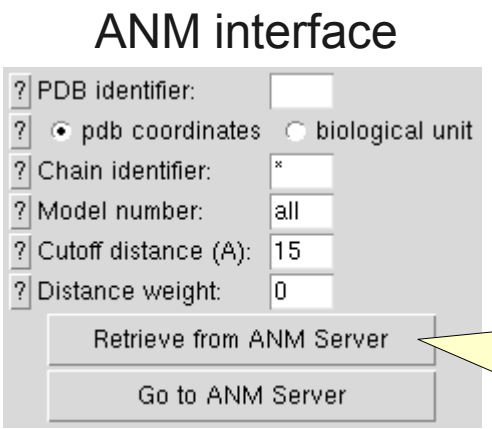
NMWiz Tutorial

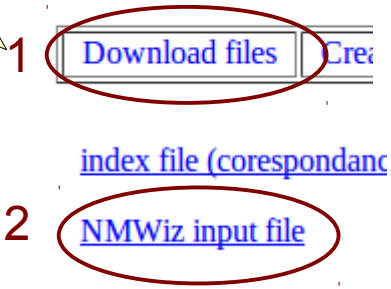
NMWiz Window Layout





An interface for submitting ANM server jobs. This button will open ANM results in a browser. NMD file needs to be downloaded from the server (works in Linux systems).

When ANM server completes your calculation, click marked links to retrieve NMD file.



Dataset GUI

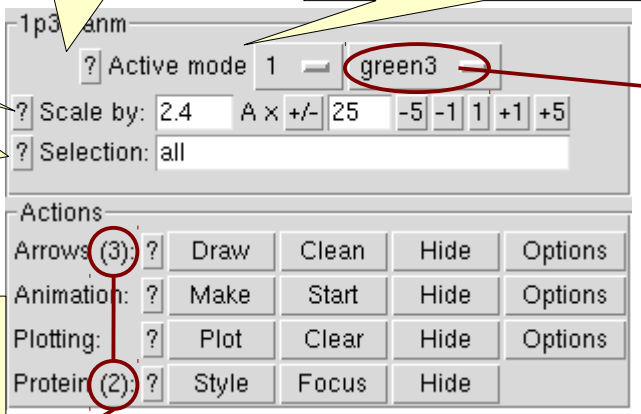
Controls to scale the length and to invert the direction of arrows

Use **?** marks to get instant help

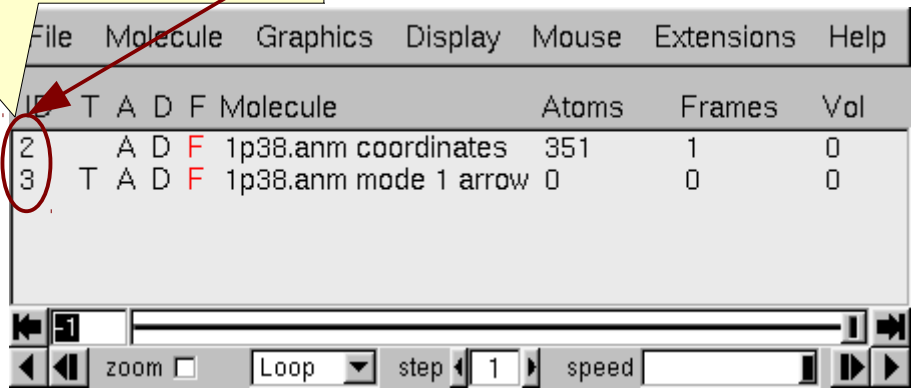
Select active mode and a color to display the arrows

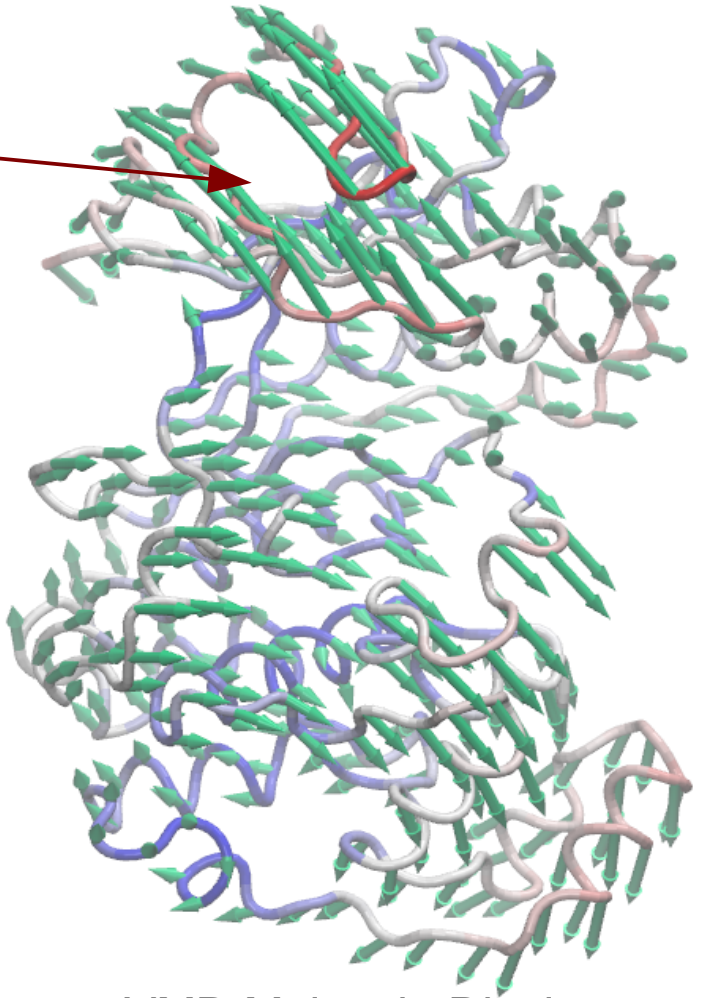
Selection string determines the residues for which the arrows will be displayed

Arrows, animations, and protein are loaded as separate molecules into VMD. Corresponding molecule ID's are shown in parentheses in NMWiz Main window.



VMD Main





VMD Molecule Display

Tip: If a molecule storing protein, arrows, or animation is deleted, NMWiz will not complain and generate another copy.

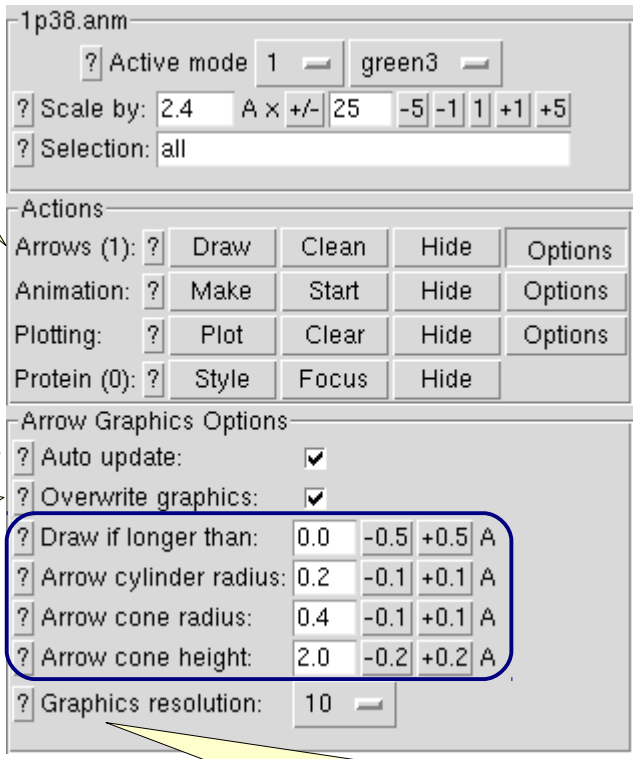
Arrows and Graphics Options

Draw: Draw/redraw arrow graphics
Clean: Remove arrow graphics (only) from the molecule whose ID is shown in parentheses
Hide/Show: Hide/Show molecule whose ID is shown in parentheses
Options: Display/hide arrow options panel

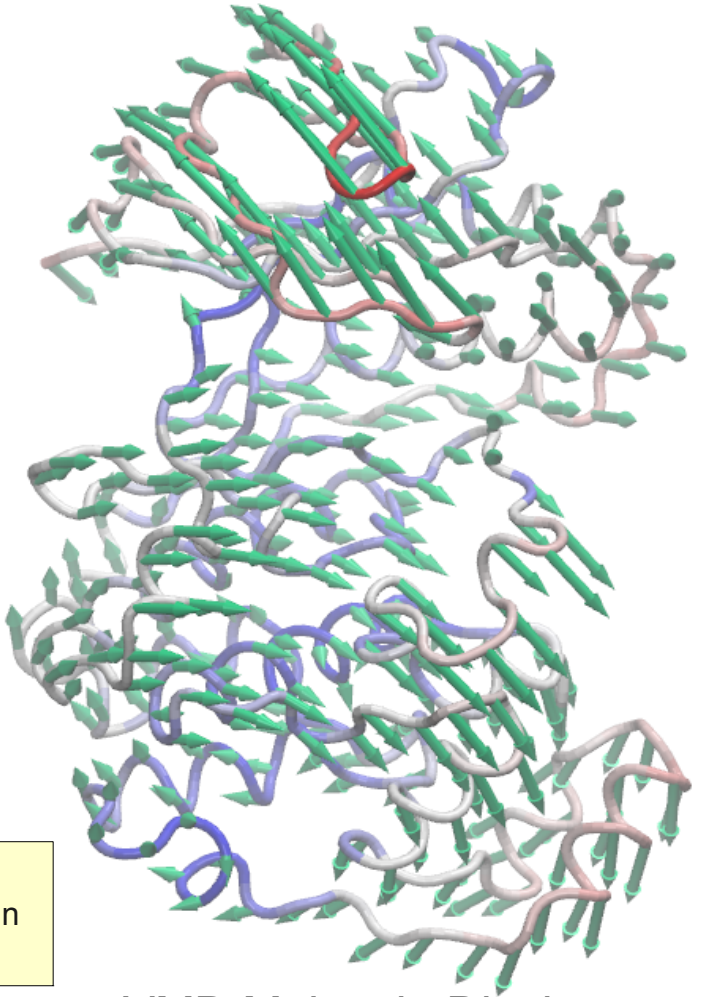
If "**Auto update**" is checked, minor tweaks in arrow graphics will be reflected to VMD view immediately

If "**Overwrite graphics**" is *not* checked, new arrow graphics will be drawn in a new molecule

Controls to fine tune arrow graphics. If "**Auto update**" is off, changes take affect after mode is redrawn.



Resolution (higher better) affects resolution of arrow graphics, and protein and animation representations



VMD Molecule Display

Tip: When working on a large molecular system drawing arrows may take seconds. Minor tweaks in arrow style will cause then to be redrawn. *Turning off* "**Auto update**" option, will avoid VMD to stall.

Another Tip: If arrow graphics show too crowded, use "**Draw if longer than**" option to draw arrows only for residues moving the specified amount (considering the scaling)

Animations and Options

Animation is a series of evenly spaced alternate configurations of a protein along a normal mode. Alternate configurations are generated by deforming the initial configuration along the active normal mode.

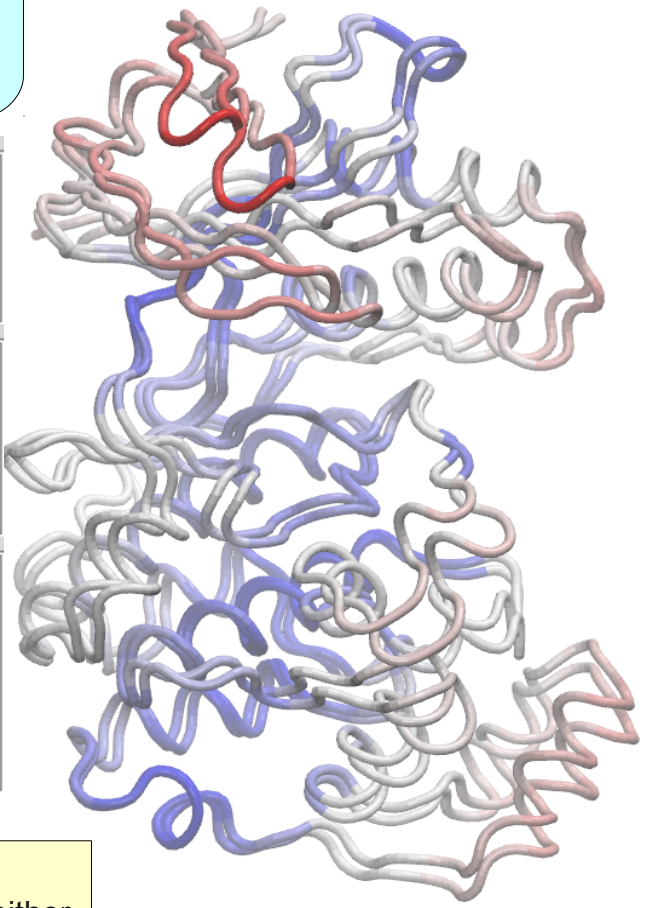
Make: Generate an animation for the active mode
Play/Pause: Play/Pause the animation
Hide/Show: Hide/Show molecule with ID shown in parentheses
Options: Display/hide animation options panel

If "**Auto animate**" is checked, an animation will be generated when the active mode is changed

If "**Overwrite animation**" is *not* checked, new animation will be loaded into a new molecule

If "**Keep trajectory file**" is checked, animation coordinates will be saved in a multi model PDB file. Example name is 1p38_anm_mode_1_animation.pdb

If "**Continuous autoplay**" is checked, animation will start playing immediately



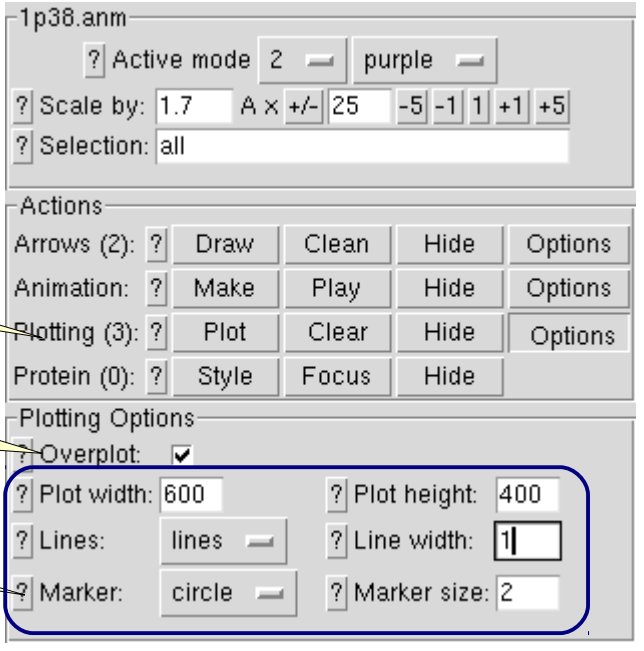
Number of frames to generate for the animation. Half of this many frames along either direction of the mode will be generated.

Plotting and Options

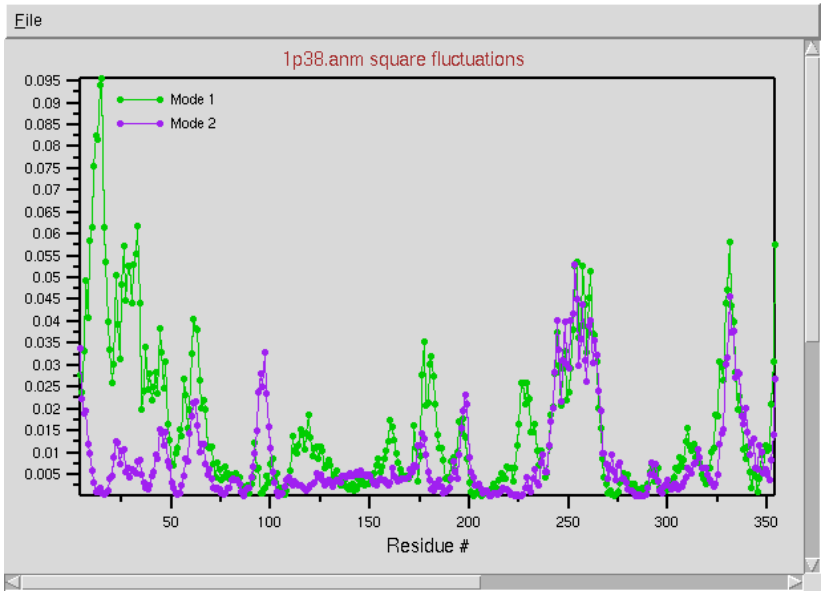
Plot: Plot square-fluctuations for the active mode
Clear: Clear selected residues (see also next slide)
Hide/Show: Hide/Show selected residues
Options: Display/hide plotting options panel

If "**Overplot**" is checked, new plots will show in the most recent window

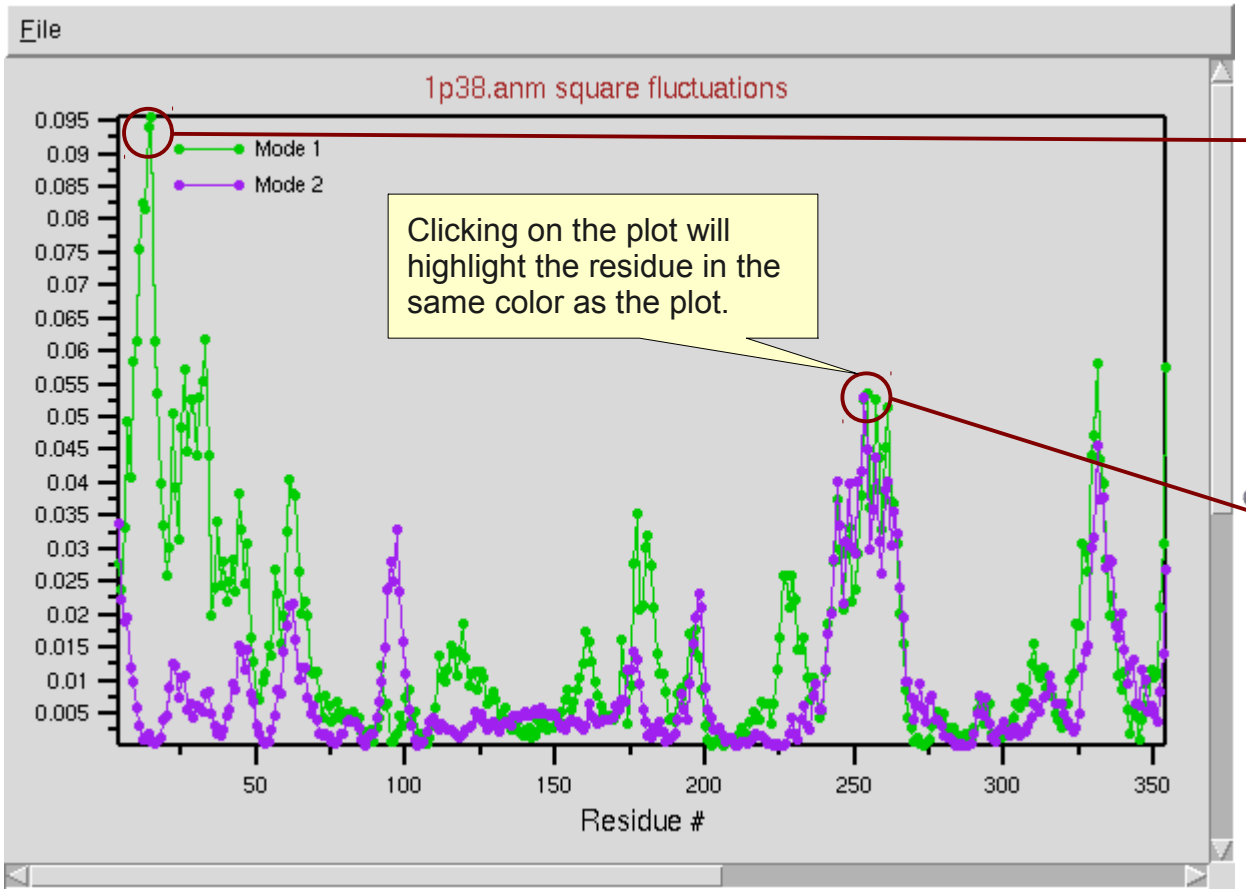
Adjust plot options

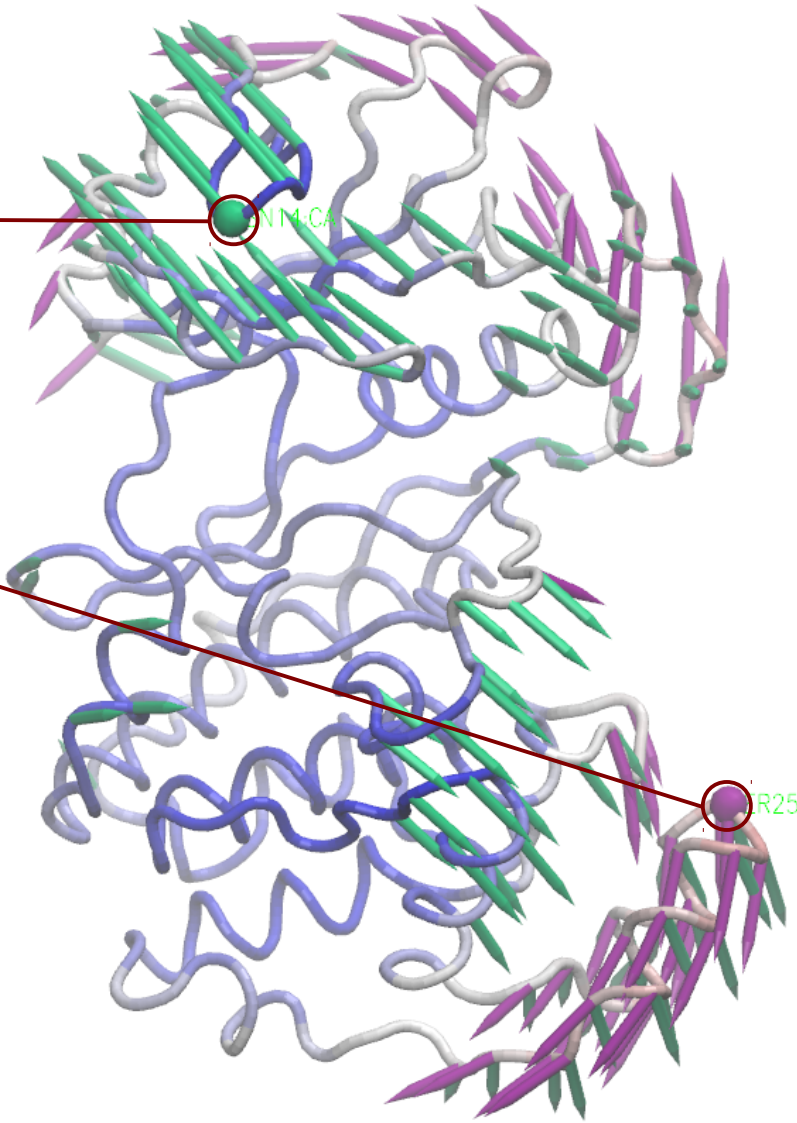


NMWiz is using a modified version of **MultiPlot** plugin of VMD:
http://www.ks.uiuc.edu/Research/vmd/plugins/multiplot/



Selecting Residues from Plots





Normal Mode Data (NMD) format

A normal mode data (**NMD**) file contains atom names, residue names/numbers, chain identifiers, b-factors, and coordinates in addition to normal modes.

Each line starts with a keyword. All recognized keywords are shown below. Number of items following a keyword must match number of atoms (N) or 3N.

```
keyword item1 item2 item3 ...
```

Name (optional) is used to identify the dataset.

Atom **coordinates** (a 3N array of numbers, where N is the number of atoms) is written in a single line. Number of atoms in a model is determined from its size. Correctness of other lines are determined based on the size of this array. That is, the size of mode arrays must match the size of the coordinate array.

Optional data

Required data

Atomic properties are optional. Their length must match number of atoms in the model.

B-factors (optional) are used for coloring protein.

```
name 1p38.anm
atomnames CA CA CA ...
resnames GLU ARG PRO ...
chainids A A A ...
resids 4 5 6 ...
bfactors 69.99 59.83 47.29 ...
coordinates 27.552 4.354 23.629 24.179 4.807 21.907 21.218 2.742 20.697 ...
mode 1 2.36 0.039 0.009 0.058 0.038 -0.011 0.052 0.043 -0.027 0.058 ...
mode 2 1.73 -0.045 -0.096 -0.009 -0.040 -0.076 -0.010 -0.049 -0.062 -0.009 ...
mode 3 1.70 0.007 -0.044 0.080 0.015 -0.037 0.062 0.012 -0.032 0.049 0.034 ...
mode 4 1.12 0.010 0.024 0.003 0.007 0.017 0.004 0.010 0.012 0.003 ...
mode 5 1.03 0.006 0.010 0.025 0.007 0.003 0.017 0.007 -0.004 0.010 ...
mode 6 0.99 -0.063 -0.066 0.060 -0.054 -0.045 0.049 -0.064 -0.033 0.053 ...
...
```

Normal mode **indices** (*optional*) are used to identify normal modes.

Mode **scaling factors** (*optional*) are used to scale mode arrows relative to each other. Scaling factor is the square-root of the inverse eigenvalue in ANM or is the square-root of eigenvalue in PCA.

Normal mode array (size 3N) is written in one line.

Linux Console Trick

```
#!/usr/local/bin/vmd -e
nmwiz_load name_of_this_file.nmd
name 1p38.anm
atomnames CA CA CA ...
resnames GLU ARG PRO ...
chainids A A A ...
resids 4 5 6 ...
bfactors 69.99 59.83 47.29 ...
coordinates 27.552 4.354 23.629 24.179 4.807 21.907 21.218 2.742 20.697 ...
mode 1 2.36 0.039 0.009 0.058 0.038 -0.011 0.052 0.043 -0.027 0.058 ...
mode 2 1.73 -0.045 -0.096 -0.009 -0.040 -0.076 -0.010 -0.049 -0.062 -0.009 ...
mode 3 1.70 0.007 -0.044 0.080 0.015 -0.037 0.062 0.012 -0.032 0.049 0.034 ...
mode 4 1.12 0.010 0.024 0.003 0.007 0.017 0.004 0.010 0.012 0.003 ...
mode 5 1.03 0.006 0.010 0.025 0.007 0.003 0.017 0.007 -0.004 0.010 ...
mode 6 0.99 -0.063 -0.066 0.060 -0.054 -0.045 0.049 -0.064 -0.033 0.053 ...
...
```

This line tells Linux shell what program to use to run the file

This line invokes NMWiz to load contents of this file

In Linux, the following will enable loading the file from the console.

```
abakan@orko:~$ vmd -e name_of_this_file.nmd
```

```
abakan@orko:~$ chmod +x name_of_this_file.nmd
abakan@orko:~$ ./name_of_this_file.nmd
```