Visualization with UCSF Chimera

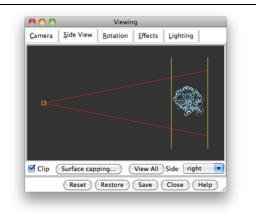
Exercise 0: Mousing and manipulating the view

0a: Mouse

Left drag = rotate
Middle (or Alt/Option) drag = move
Right (or two-finger) drag = zoom
Scroll wheel or two-finger swipe = zoom quickly

Ctrl-Left Click = select/deselect Shift-Ctrl-Left Click = add to selection

Slab: "Favorites > Side View"



Ob: Center of view and rotation

Zoom to the selection: "Actions > Focus"

Rotate about the selection: "Actions > Set Pivot" or Ctrl-Left Double Click and select "Set Pivot". TIP: If nothing is selected, "Focus" and "Set Pivot" revert to the whole.

TIP: More on selections in Exercise 4.

Exercise 1: Morphing and Movies

Adapted from http://www.cgl.ucsf.edu/chimera/tutorials/movies08/moviemaking.html

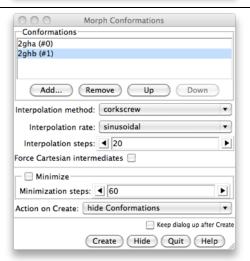
Load the start and end points, delete crystallographic dimers, and overlap them

- 1. Fetch "2gha" and "2ghb": "File > Fetch by ID..."
- "Select > Chain > C" then "Actions > Atoms/Bonds > delete".
- 3. "Select > Chain > B > all" then "Actions > Atoms/Bonds > delete".
- 4. Show the MatchMaker panel: "Tools > Structure Comparison > MatchMaker"
- 5. Click on "2gha" in the "Reference structure" box and click "OK".

Reference structure: Structure(s) to match 2gha (#0) 2ghb (#1) 2gha (#0) 2ghb (#1) Further restrict matching to current selection Further restrict matching to current selection Chain pairing Best-aligning pair of chains between reference and match structure O Specific chain in reference structure with best-aligning chain in match structure Alignment algorithm: Needleman-Wunsch Matrix: BLOSUM-62 Gap extension penalty 1 ✓ Include secondary structure score (30%) Show parameters ✓ Compute secondary structure assignments Show pairwise alignment(s) -Matching-✓ Iterate by pruning long atom pairs until no pair exceeds: After superposition, compute structure-based multiple sequence alignment Save settings OK Apply Cancel Help

Compute the morph

- 1. Access the "Tools > Structure Comparison > Morph Conformations" panel.
- 2. Change "Interpolation rate" to "sinusoidal" and "Action on Create" to "hide Conformations"
- 3. Click "Add..." to add the first and second conformation. Then click "Create" and wait a few seconds. A new window and the morph should appear.



Output the movie

1. Click the Play button to view the movie. Save the movie with "File > Record Movie..."

TIP: Images and movies are rendered at the size of the 3D window unless specified otherwise. Movies benefit from using a specific frame size. Set the frame size by setting the size of the 3D window:

- 1. Access the command line: "Favorites > Command Line"
- 2. Type "windowsize 640 480"

