

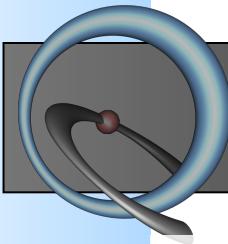
RBVI

# An Introduction to Molecular Visualization with UCSF Chimera

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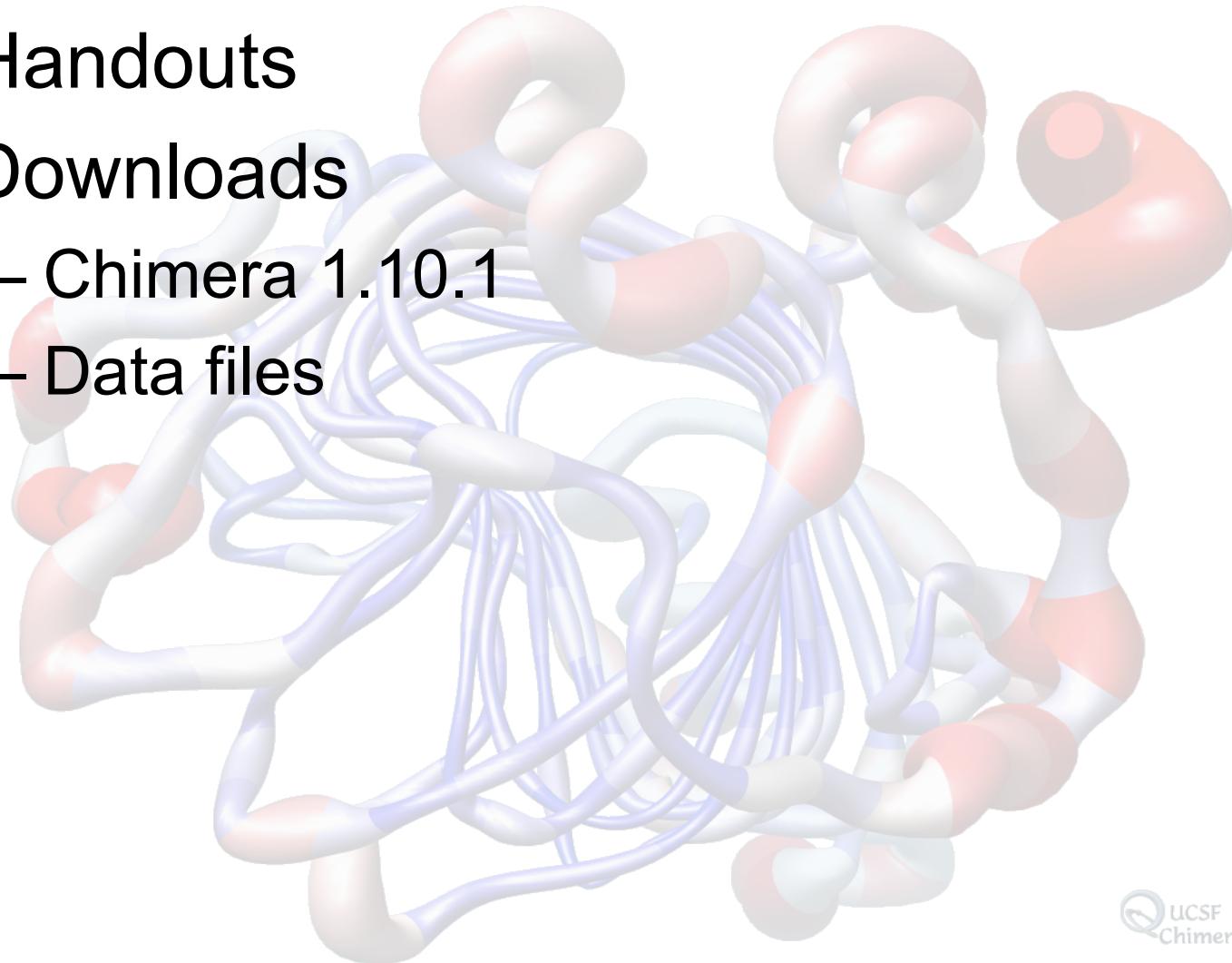
University of California, San Francisco



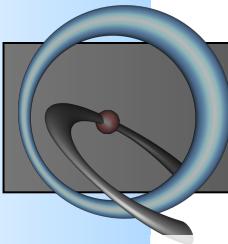


# Materials

- Handouts
- Downloads
  - Chimera 1.10.1
  - Data files

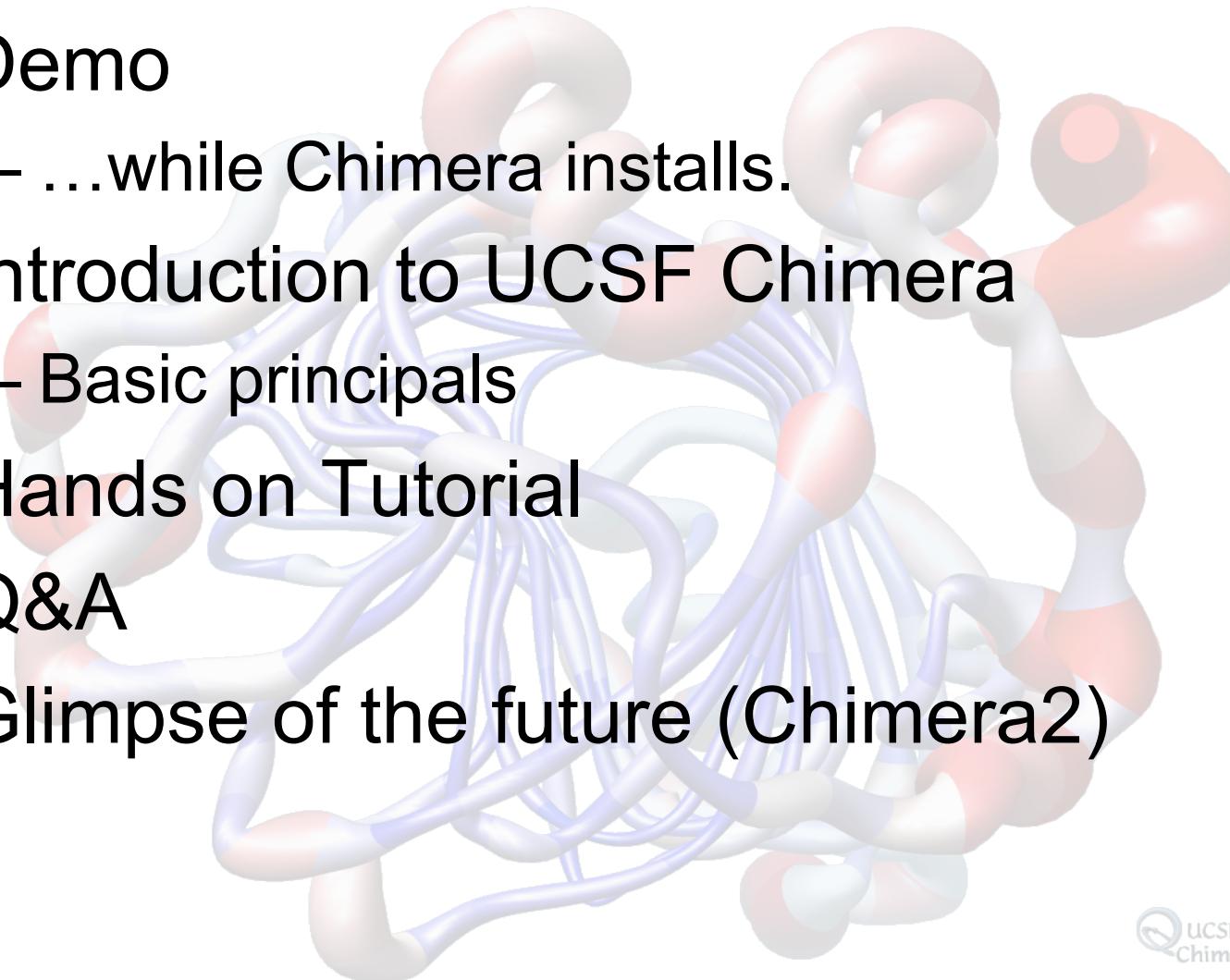


UCSF  
Chimera

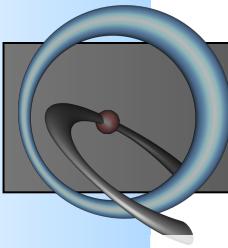


# Agenda

- Demo
  - ...while Chimera installs.
- Introduction to UCSF Chimera
  - Basic principals
- Hands on Tutorial
- Q&A
- Glimpse of the future (Chimera2)

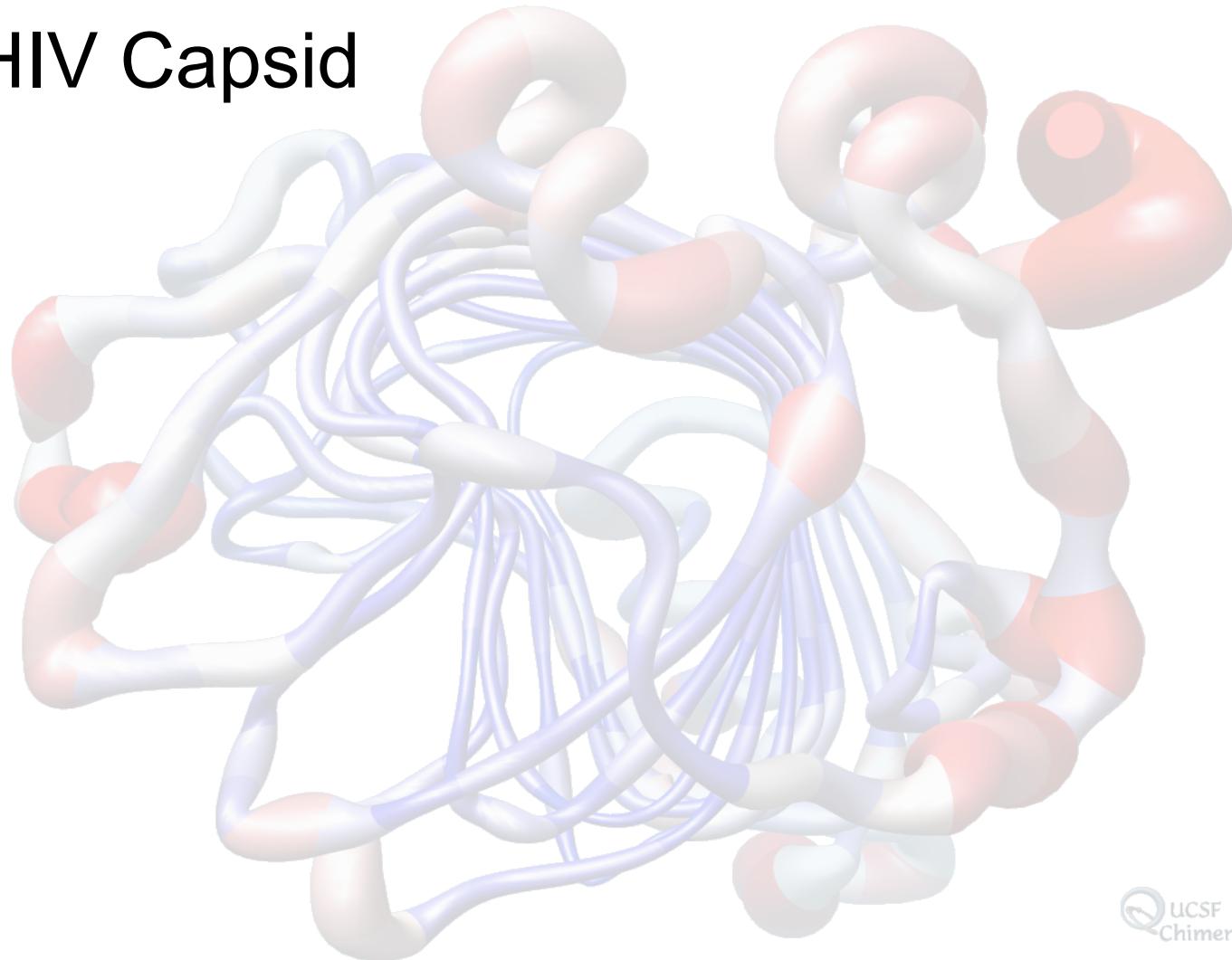


UCSF  
Chimera

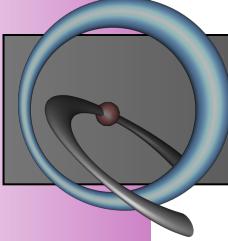


# Demo

- HIV Capsid



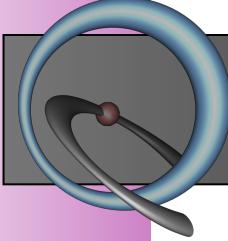
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Chimera



# UCSF Chimera



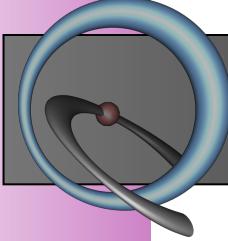
- Target audience
  - Scientists who need to analyze and model molecular systems in some detail
  - Scientists who want to develop new analytical methods
  - Scientists or educators who wish to communicate biological concepts visually
- Organization
  - Core features
  - Additional tools



# Chimera Core Features

UCSF  
Chimera

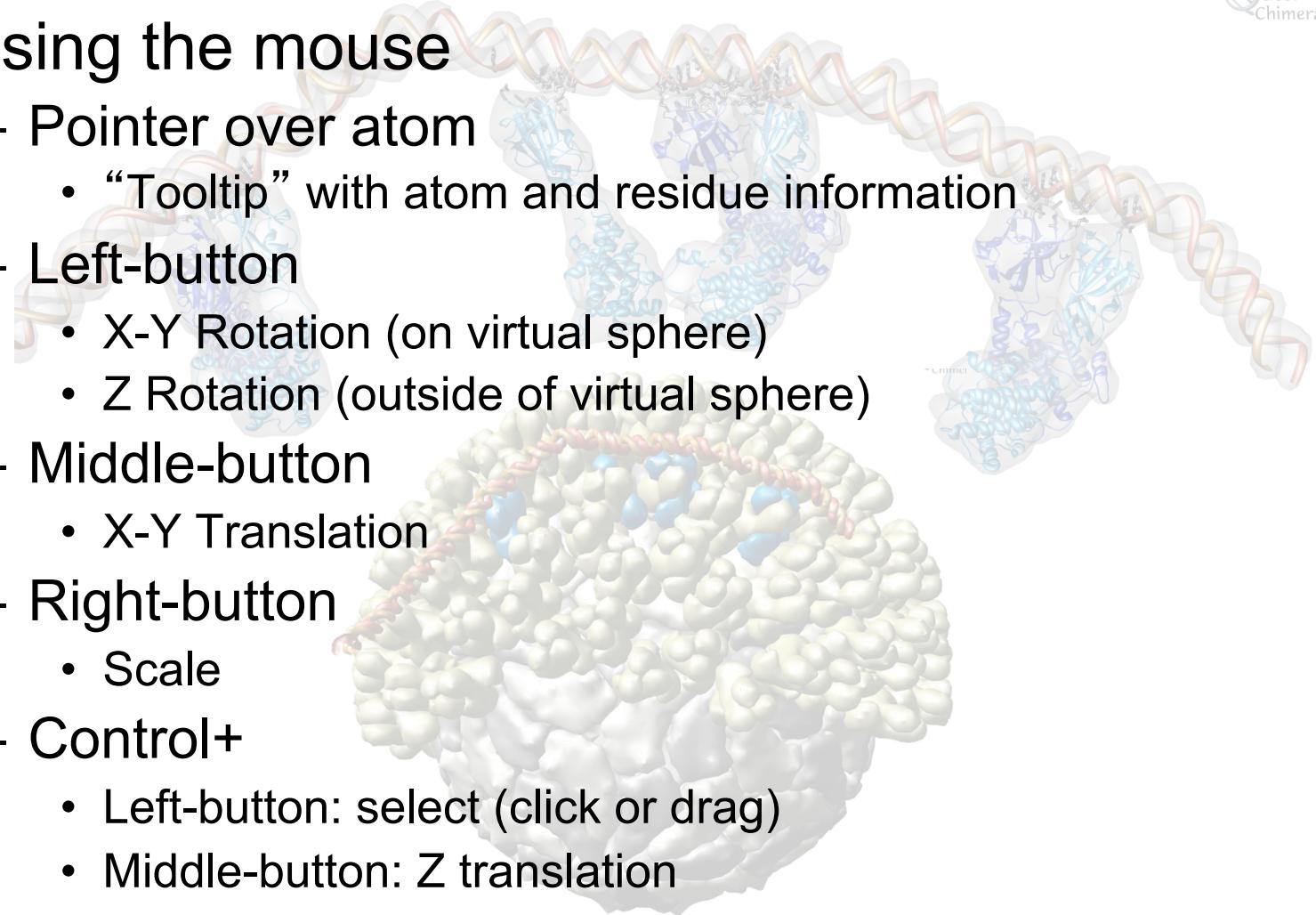
- Concepts
  - Graphical manipulation
  - Chemical knowledge
    - Hierarchy: Model→Chain→Residue→Atom
    - Attributes available at model, residue, and atom levels
  - Selection - Action
  - GUI/Command-line equivalence
    - For core, not necessarily extensions

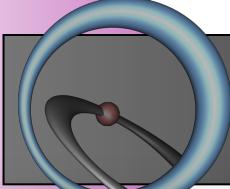


# Core Features (cont.)

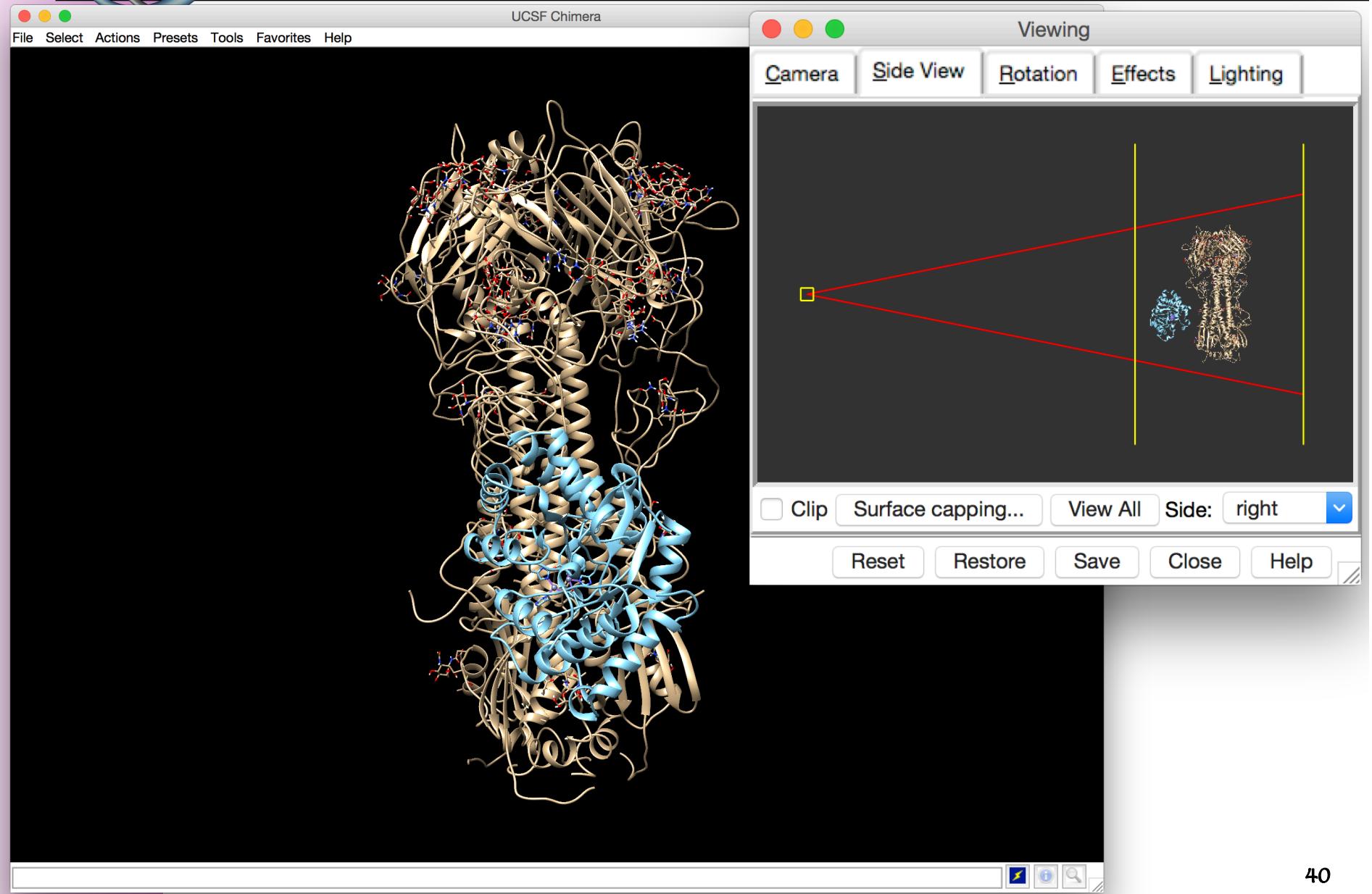
UCSF  
Chimera

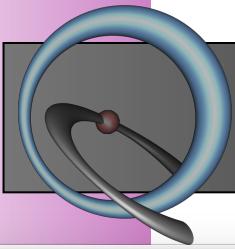
- Using the mouse
  - Pointer over atom
    - “Tooltip” with atom and residue information
  - Left-button
    - X-Y Rotation (on virtual sphere)
    - Z Rotation (outside of virtual sphere)
  - Middle-button
    - X-Y Translation
  - Right-button
    - Scale
  - Control+
    - Left-button: select (click or drag)
    - Middle-button: Z translation





# Core Features (cont.)





# Core Features (cont.)

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Inspect Selection

Selected:  
1 molecule model  
7 residues  
52 atoms  
51 bonds

Inspect Molecule model

active: true  
aromatic color: No  
aromatic display: false  
aromatic line style:   
aromatic ring style: disk  
auto-chaining: on  
ball scale: 0.25  
color:   
displayed: true  
line style:   
line width: 1.0  
residue label positioning: centroid  
ribbon (cardinal) smoothing: none  
ribbon (cardinal) stiffness: 0.8  
ribbon hides backbone atoms: true  
ribbon inside color: No  
ribbon spline: B-spline  
silhouette: true  
stick scale: 1.0  
surface color: No  
surface opacity: -1.0  
vdw density: 5.0  
vdw dot size: 1.0

52 atoms, 51 bonds Write List... Write PDB... Close Help

The image shows a 3D ribbon model of a protein structure against a black background. The main body of the protein is represented by tan-colored ribbons forming alpha-helices and beta-sheets. A smaller, more compact blue ribbon structure is located on the right side. A green stick model is partially visible at the bottom left. The UCSF Chimera interface is overlaid on the image, featuring a menu bar, a toolbar, and a large control panel on the right side titled 'Inspect Selection' and 'Inspect Molecule model'. The control panel contains numerous dropdown menus and input fields for modifying the visual representation of the selected molecule model.

# Core Features (cont.)

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Model Panel

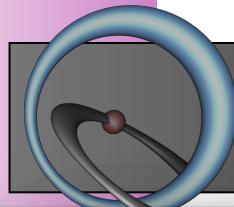
ID	Active	Shown	Name
0	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1hgg
1	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	1BF6

activate  
activate all  
activate only  
add/edit note...  
attributes...  
biological unit  
clipping...  
close  
compute SS  
copy/combine...  
deactivate  
group/ungroup  
hide  
match...  
rainbow...  
Ramachandran plot...  
rename...  
select  
select chain(s)...  
show  
show all atoms  
show only  
toggle active  
transform as...  
write PDB

favorites  all

Configure... Close Help

The image shows the UCSF Chimera software interface. On the left, a 3D ribbon model of a protein structure is displayed against a black background. The structure consists of several domains, with one domain colored blue and the others in a light beige or tan color. On the right, a 'Model Panel' window is open, listing two entries: '1hgg' and '1BF6'. Each entry has three checkboxes: 'Active' (checked), 'Shown' (checked), and 'Name' (unchecked). The 'Model Panel' window also contains a vertical list of various actions and tools. At the bottom of the panel are radio buttons for 'favorites' (selected) and 'all', and buttons for 'Configure...', 'Close', and 'Help'.



# Core Features (cont.)

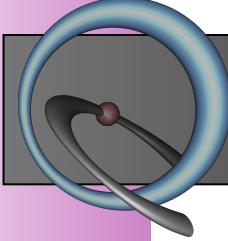
MultAlignViewer

File Edit Structure Headers Numberings Tree Info Preferences

	1	11	21	31	41
Consensus	- - - - - G f T L i	H E H L r v f s e a	v r q q w p h l y N	e D - - - e e f r n	a v n E v k r a - -
Conservation					
1BF6.1BF6_(#1)_chain_B	S F D P T G Y T L A	H E H L H I D L S G	F K N - - - - - N	V D C R L D Q Y A F	I C Q E M N D L - -
4LEF_H	S F D P T G Y T L A	H E H L H I D L S G	F K N - - - - - N	V D C R L D Q Y A F	I C Q E M N D L - -
4G2D_A	- - - - - G F T L i	H E H L R V f s E A	v R y - - - - - Q	w p h l y N E d e e	L r N a V N E V k r
4KER_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
3UF9_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
2VC7_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
4KEZ_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
4KET_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
4KF1_D	- - - - - G F T L i	H E H L R V f s E A	v R Q q w p h l y N	e D - - - E E F r n	a v N E V K r a - -
Consensus	- M q f G V k t i v	d p T v m g l G R d	i r F M e k V v k a	T G I N I V A g T G	i Y i y i d l P f y
Conservation					
1BF6.1BF6_(#1)_chain_B	- M T R G V R N V I	E M T N R Y M G R N	A Q F M L D V M R E	T G I N V V A C T G	Y Y Q D A F F P E H
4LEF_H	- M T R G V R N V I	E M T N R Y M G R N	A Q F M L D V M R E	T G I N V V A C T G	Y Y Q D A F F P E H
4G2D_A	a M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K t	T G I N L V A g T G	i Y i y V d L P f Y
4KER_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
3UF9_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
2VC7_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
4KEZ_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
4KET_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
4KF1_D	- M q f G V K T I V	D p T v m g l G R D	i R F M e k V V K a	T G I N L V A g T G	i Y i y i d L P f Y
Consensus	f l n R S i d E i A	d l f i h d l k e G	I q G T I n K A G f	v x - I a a d E p g	I T k d v E K V i r
Conservation					
1BF6.1BF6_(#1)_chain_B	V A T R S V Q E L A	Q E M V D E I E Q G	I D G T E L K A G I	I A E I G T S E G K	I T P L E E K V F I
4LEF_H	V A T R S V Q E L A	Q E M V D E I E Q G	I D G T E L K A G I	I A E I G T S E G K	I T P L E E K V F I
4G2D_A	f i N R S I D E I A	D I F I h D I K E G	I Q A T S n K A G F	V x - I A A D E p g	I T k d v E K V i r
4KER_D	f i N R S I D E I A	D I F I h D I K E G	I Q G T I n K A G F	V x - I A A D E p g	I T k d v E K V i r
3UF9_D	f i N R S I D E I A	D I F I h D I K E G	I Q G T I n K A G F	V x - I A A D E p a	I T k d v E K V i r

Alignment reformatted

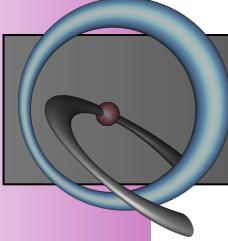
Quit Hide Help



# Core Features (cont.)

UCSF  
Chimera

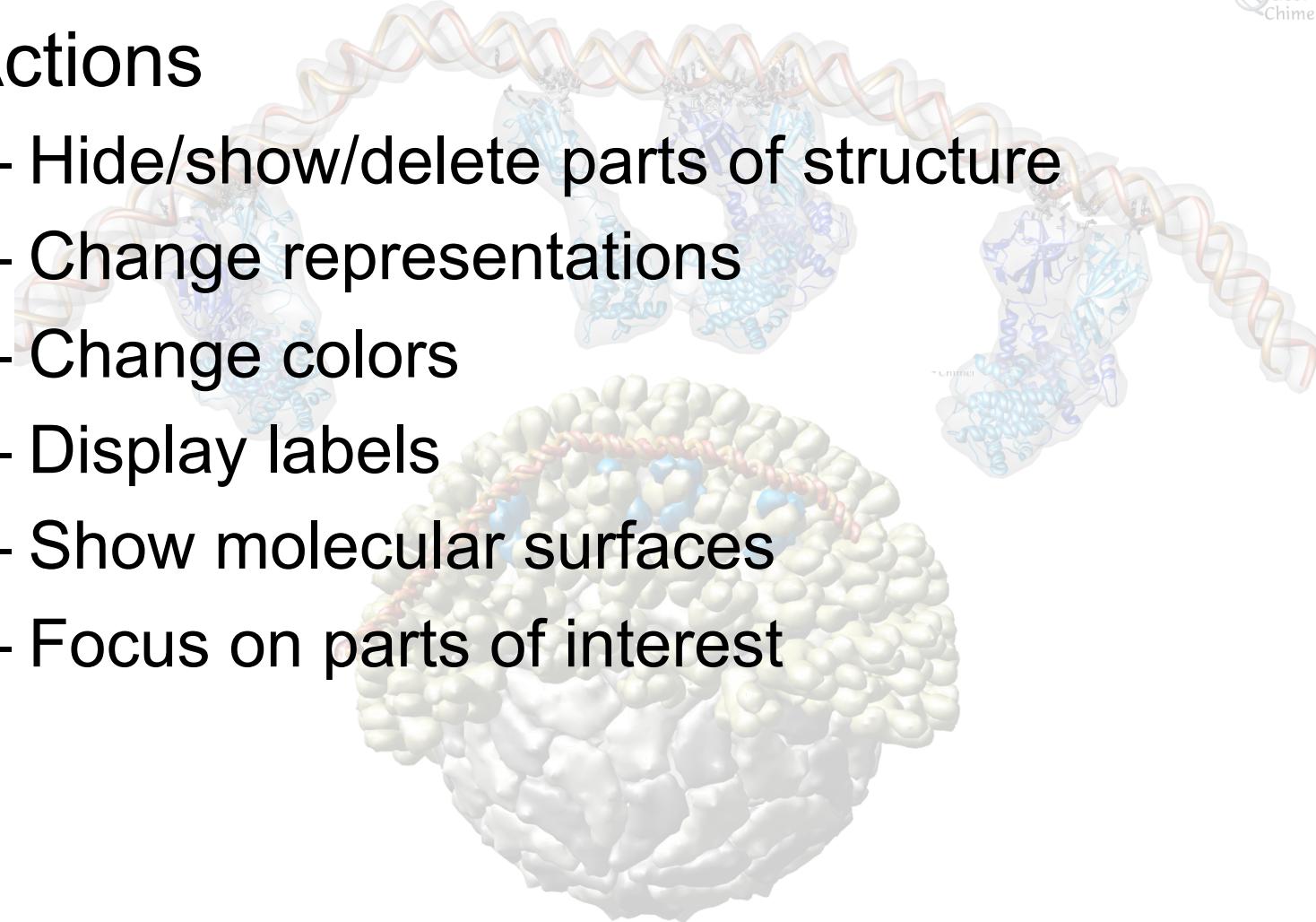
- Selection methods
  - Using mouse
    - Control-click and control-drag
    - Shift-control-click and shift-control-drag to add to selection
  - By atom and residue names and types
  - By higher order structure
    - e.g., chains, ligands, solvent
  - By spatial location
    - e.g., within some distance of another selection
  - By attribute values
    - e.g., temperature factor, occupancy
  - Can extend any selection with up-arrow: ↑
  - NOTE: by default, if nothing is selected, everything is selected

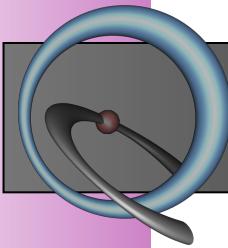


# Core Features (cont.)

- Actions
  - Hide/show/delete parts of structure
  - Change representations
  - Change colors
  - Display labels
  - Show molecular surfaces
  - Focus on parts of interest

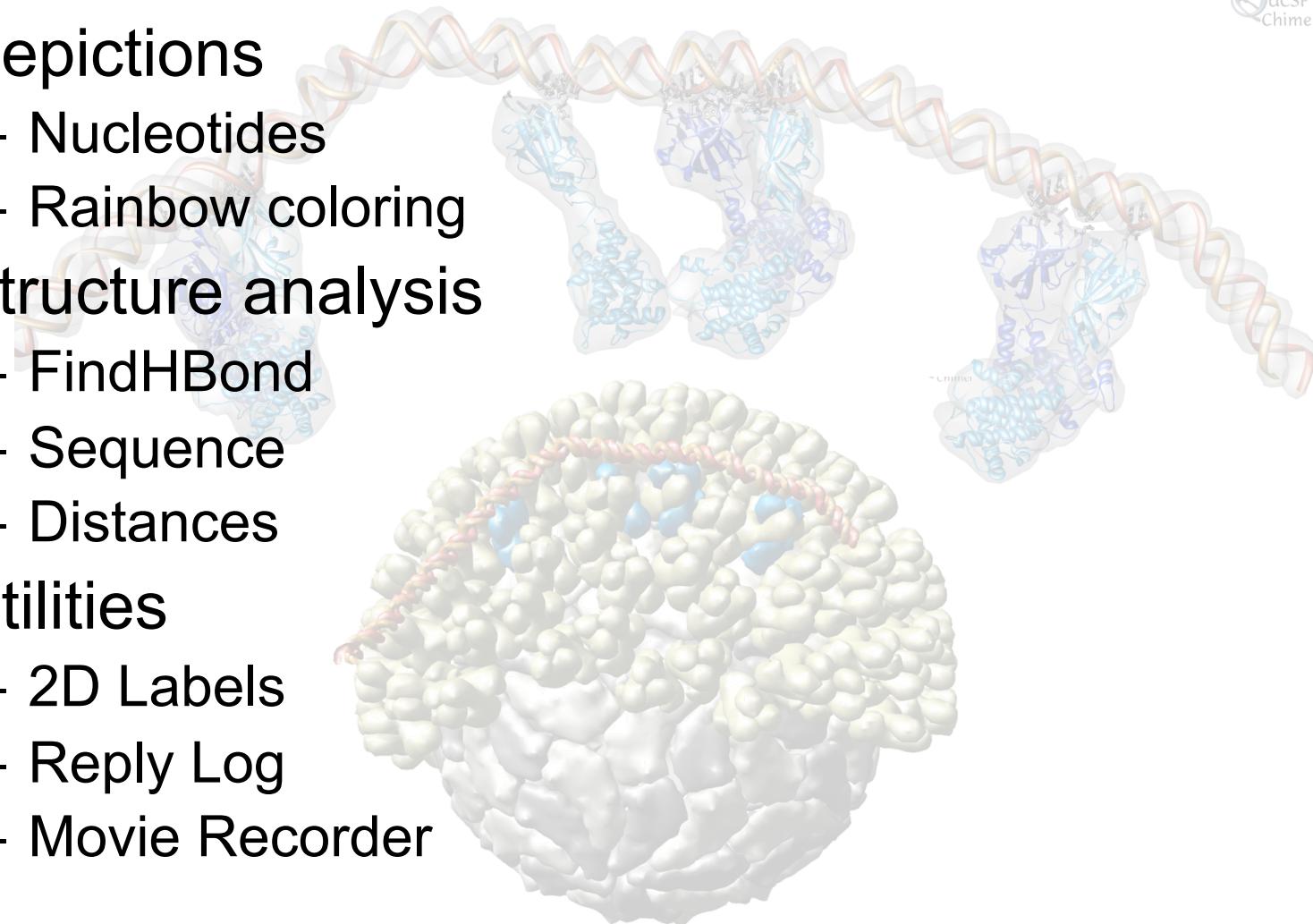
UCSF  
Chimera

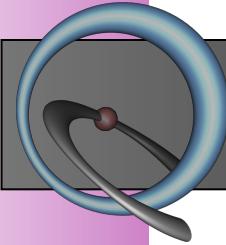




# Commonly used tools

- Depictions
  - Nucleotides
  - Rainbow coloring
- Structure analysis
  - FindHBond
  - Sequence
  - Distances
- Utilities
  - 2D Labels
  - Reply Log
  - Movie Recorder





# Questions?

- Anything you want to see in particular?

UCSF  
Chimera

