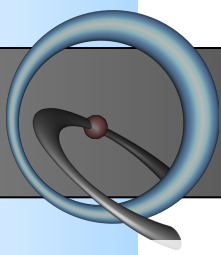


An Introduction to Molecular Visualization with UCSF Chimera

John “Scooter” Morris, Ph.D.
scooter@cgl.ucsf.edu

University of California, San Francisco

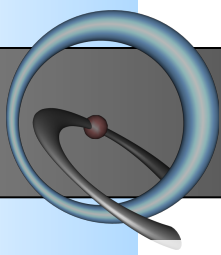


Introductions

- About me

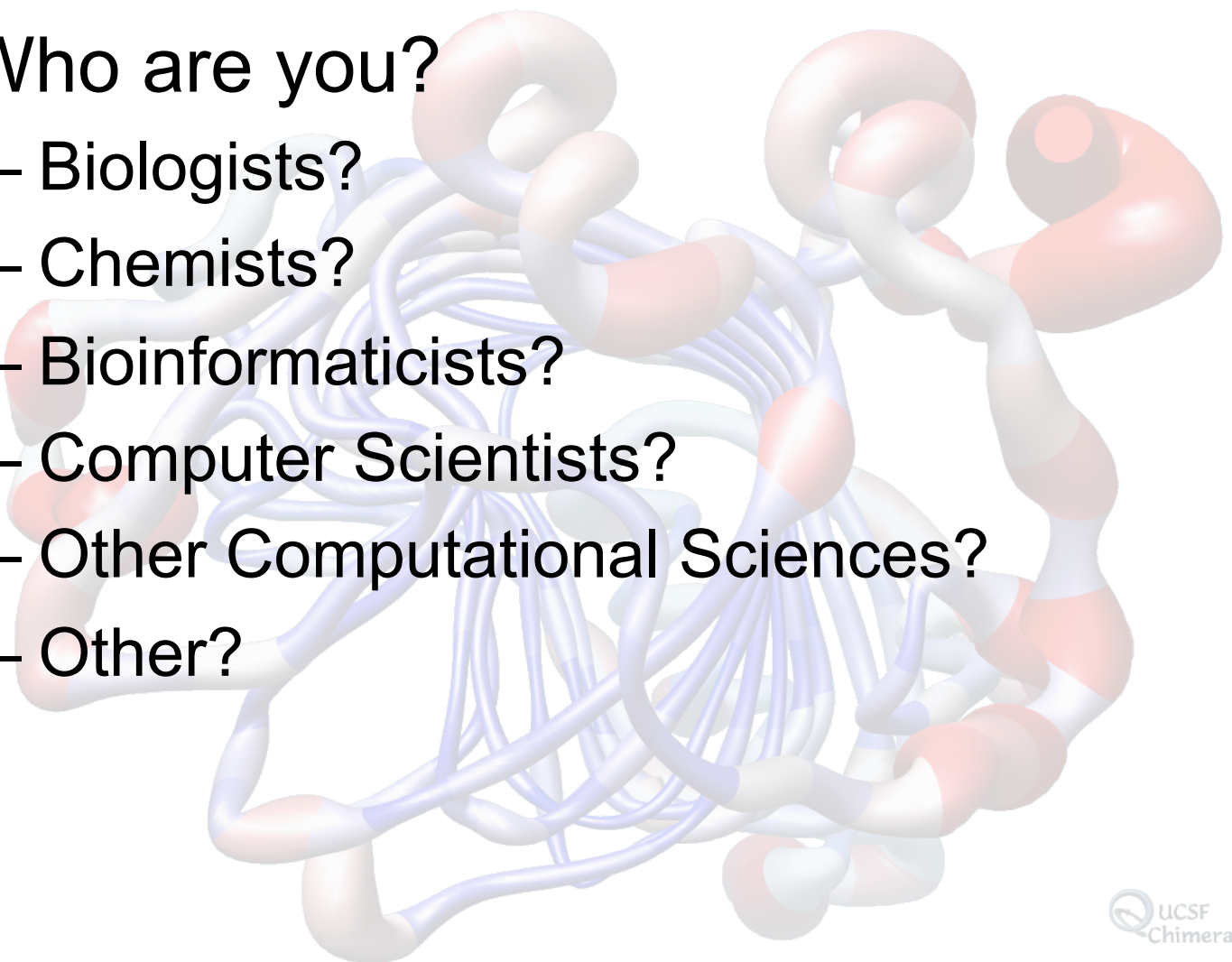
- John “Scooter” Morris:

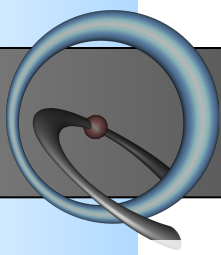
- RBVI Executive Director
 - Adjunct Professor, Department of Pharmaceutical Chemistry, UCSF
 - 19 years in pharmaceutical industry (Genentech)
 - 11 years at RBVI



Introductions

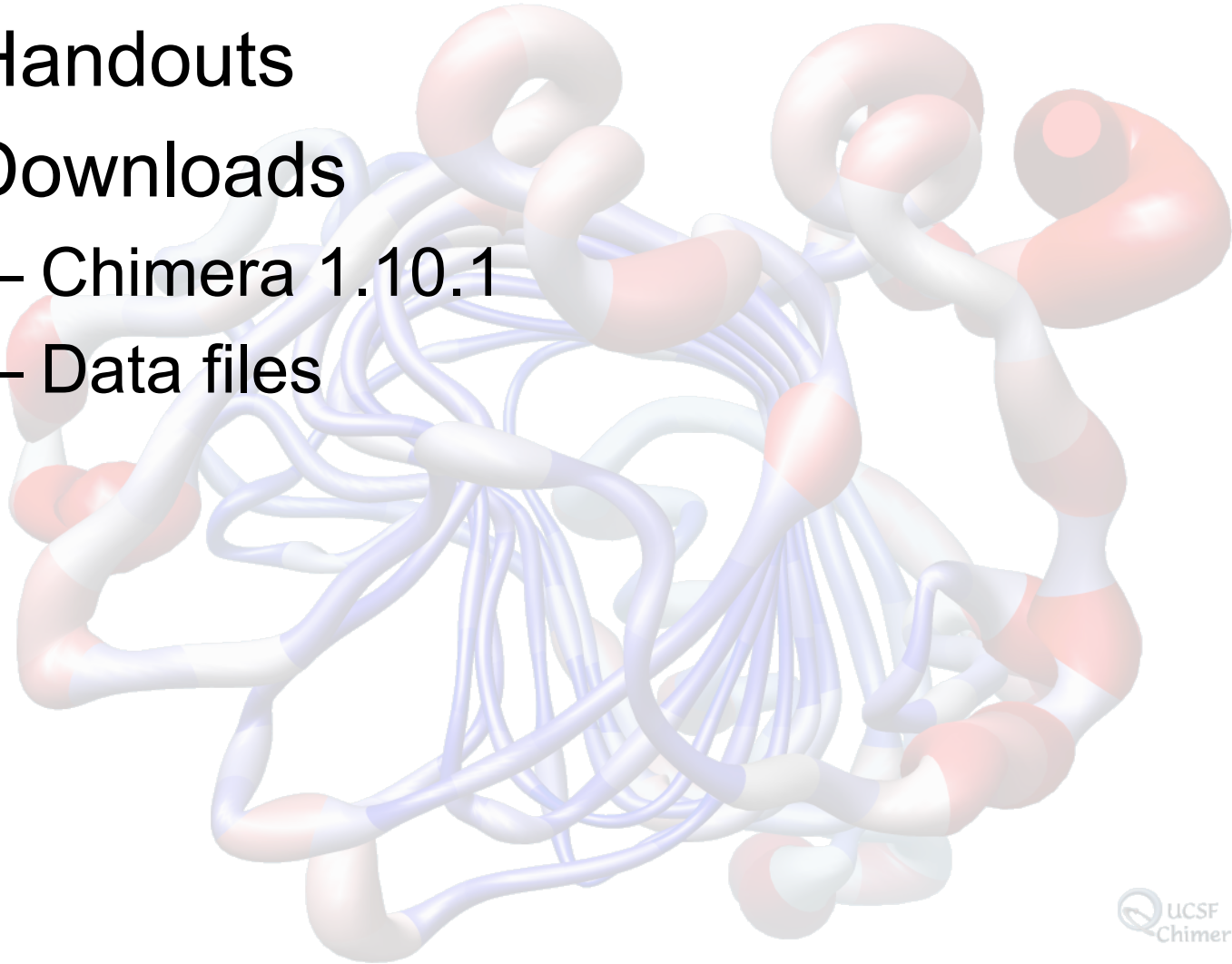
- Who are you?
 - Biologists?
 - Chemists?
 - Bioinformaticists?
 - Computer Scientists?
 - Other Computational Sciences?
 - Other?

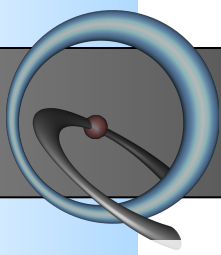




Materials

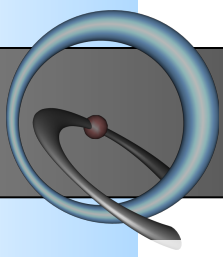
- Handouts
- Downloads
 - Chimera 1.10.1
 - Data files





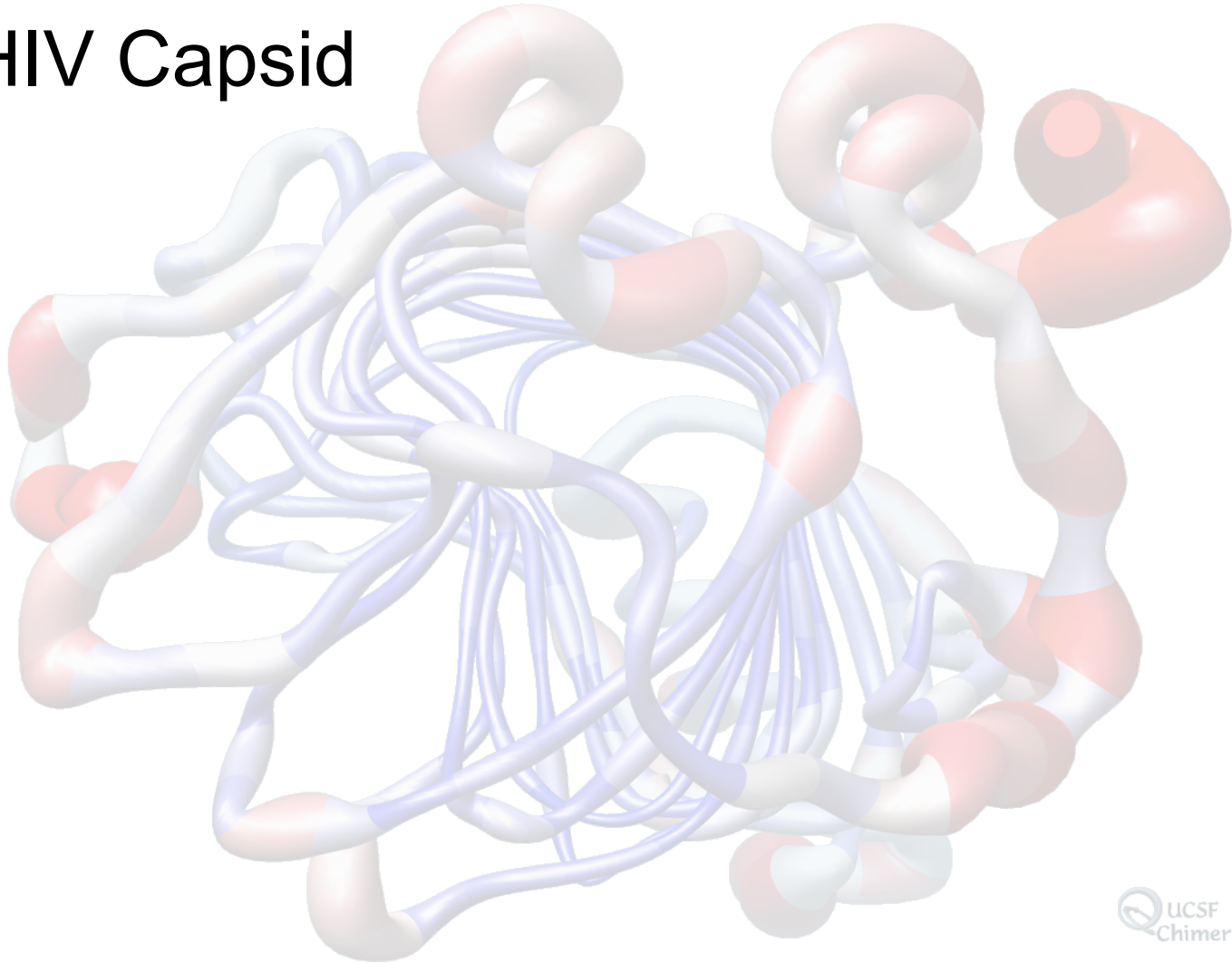
Agenda

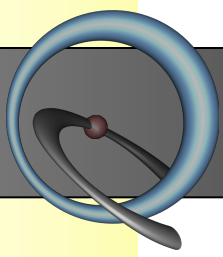
- Demo
 - ...while Chimera installs.
- Introduction to UCSF Chimera
 - Basic principals
- Hands on Tutorial
- Q&A
- Glimpse of the future (Chimera2)



Demo

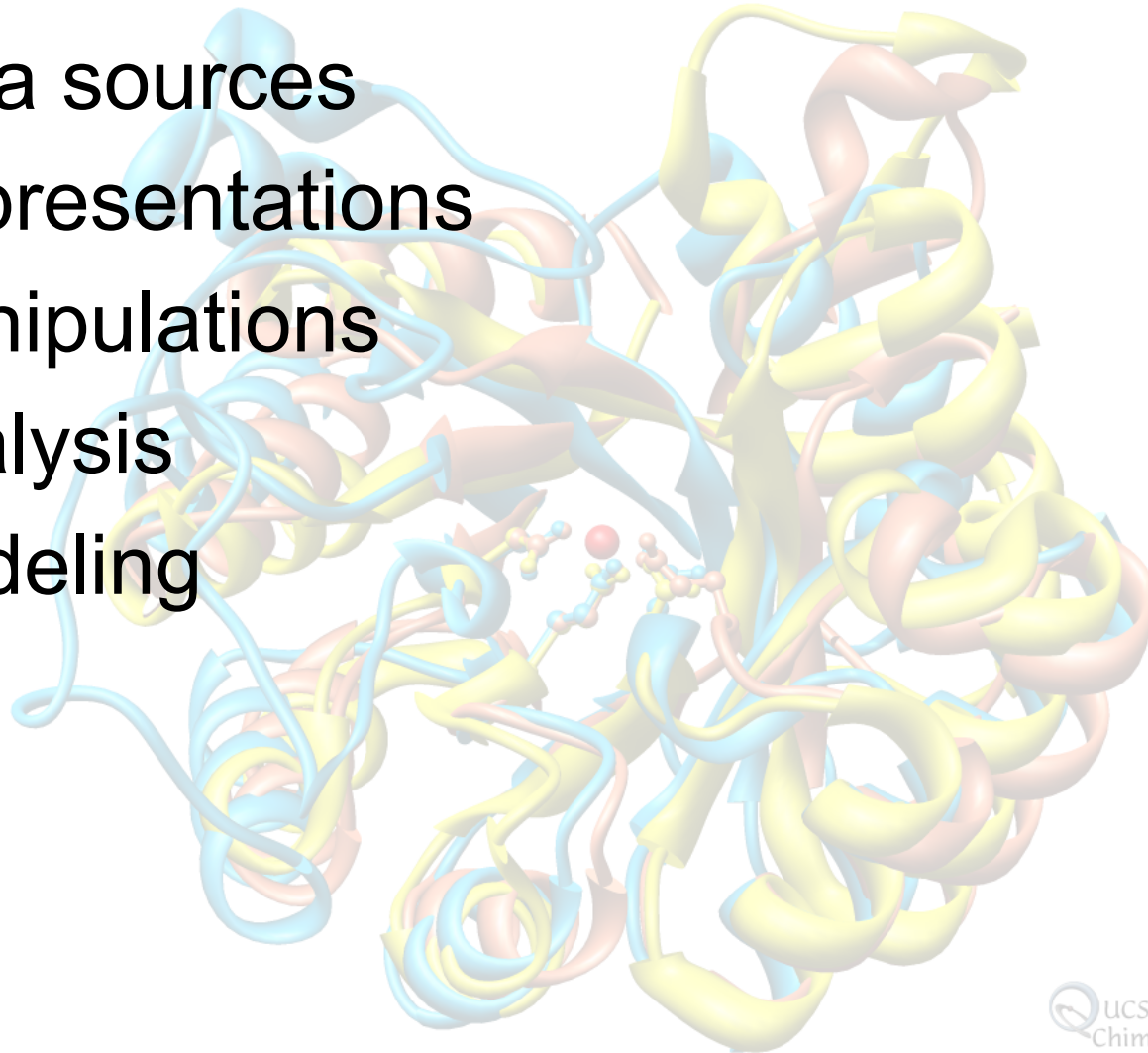
- HIV Capsid

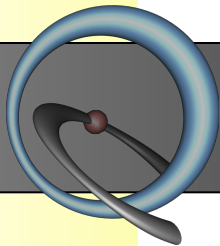




Molecular Visualization

- Data sources
- Representations
- Manipulations
- Analysis
- Modeling





Definitions

- modeling (model):

Function: *verb*

transitive verb

1 : to plan or form after a pattern : [SHAPE](#)

3 b : to produce a representation or simulation of <using a computer to *model* a problem>

4 : to construct or fashion in imitation of a particular model <*modeled* its constitution on that of the United States>

intransitive verb

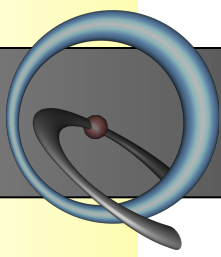
1 : to design or imitate forms : make a pattern <enjoys *modeling* in clay>

- visualization:

Function: *noun*

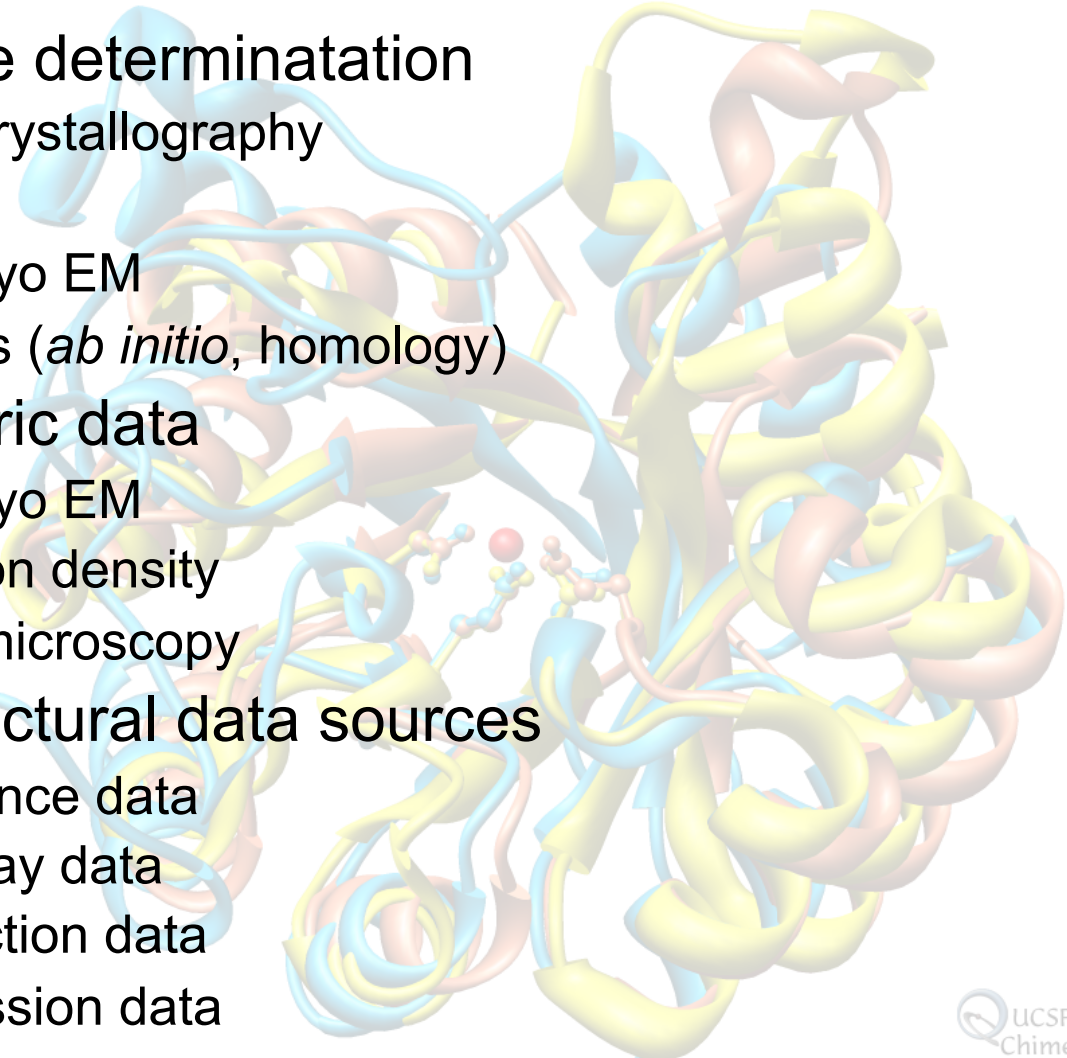
1 : formation of mental [visual](#) images

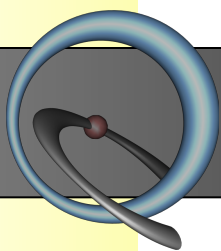
2 : the act or process of interpreting in [visual](#) terms or of putting into visible form



Data sources

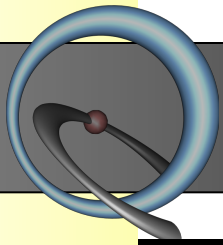
- Structure determination
 - Xray crystallography
 - NMR
 - EM/Cryo EM
 - Models (*ab initio*, homology)
- Volumetric data
 - EM/Cryo EM
 - Electron density
 - Light microscopy
- Non-structural data sources
 - Sequence data
 - Pathway data
 - Interaction data
 - Expression data



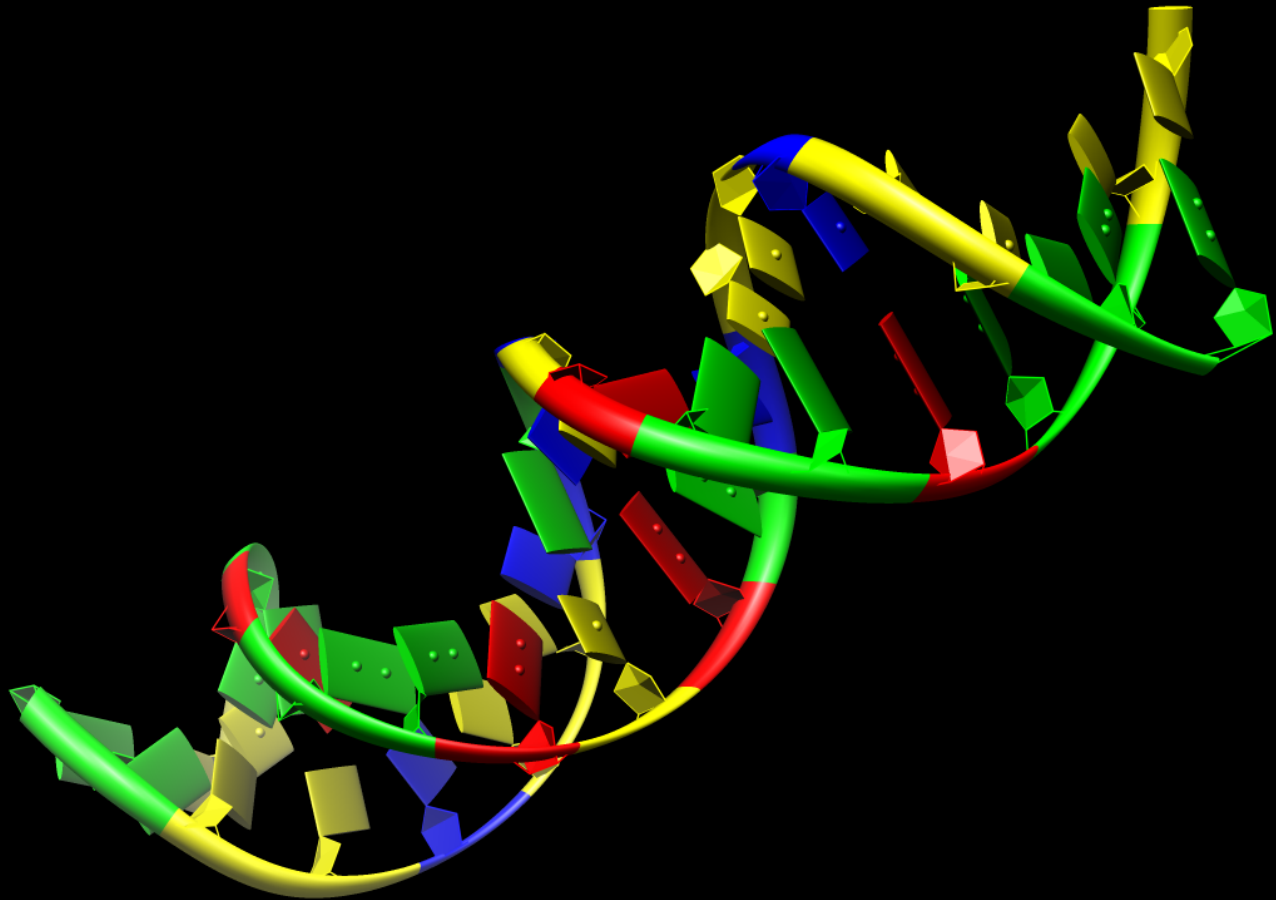


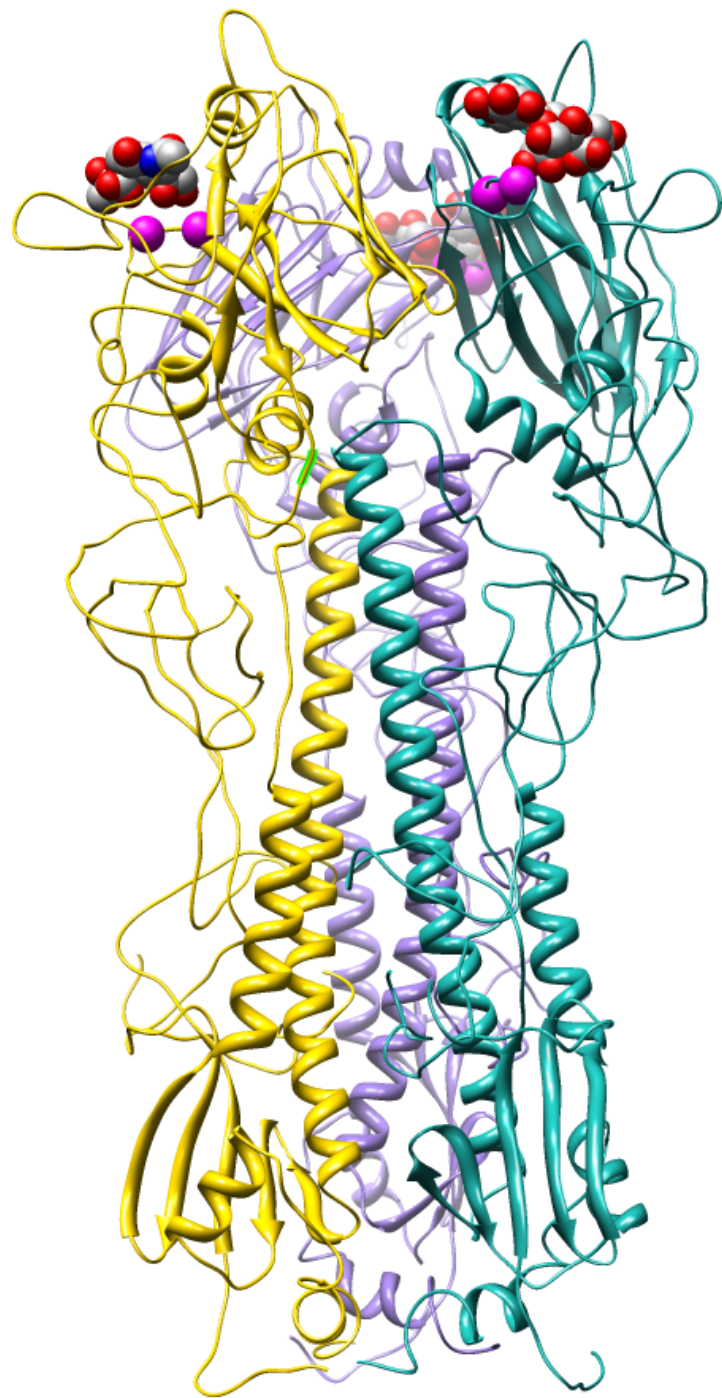
Data sources

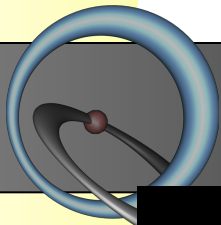
- Structure repositories
 - Protein Databank: <http://www.rcsb.org/>
 - Nucleic Acid Database (NDB): <http://ndbserver.rutgers.edu/>
 - Structural Classification of Proteins (SCOP):
<http://scop.mrc-lmb.cam.ac.uk/scop/>
 - ModBase: <http://modbase.compbio.ucsf.edu/>
 - Cambridge Structural Database (CSD):
<http://www.ccdc.cam.ac.uk/products/csd/>
 - VIPER EM Database: <http://mmtsb1.scripps.edu/emdb/>
 - EM Database: <http://www.ebi.ac.uk/msd-srv/emsearch/index.html>
 - Uppsala Electron Density Server: <http://eds.bmc.uu.se/eds/>



Representations

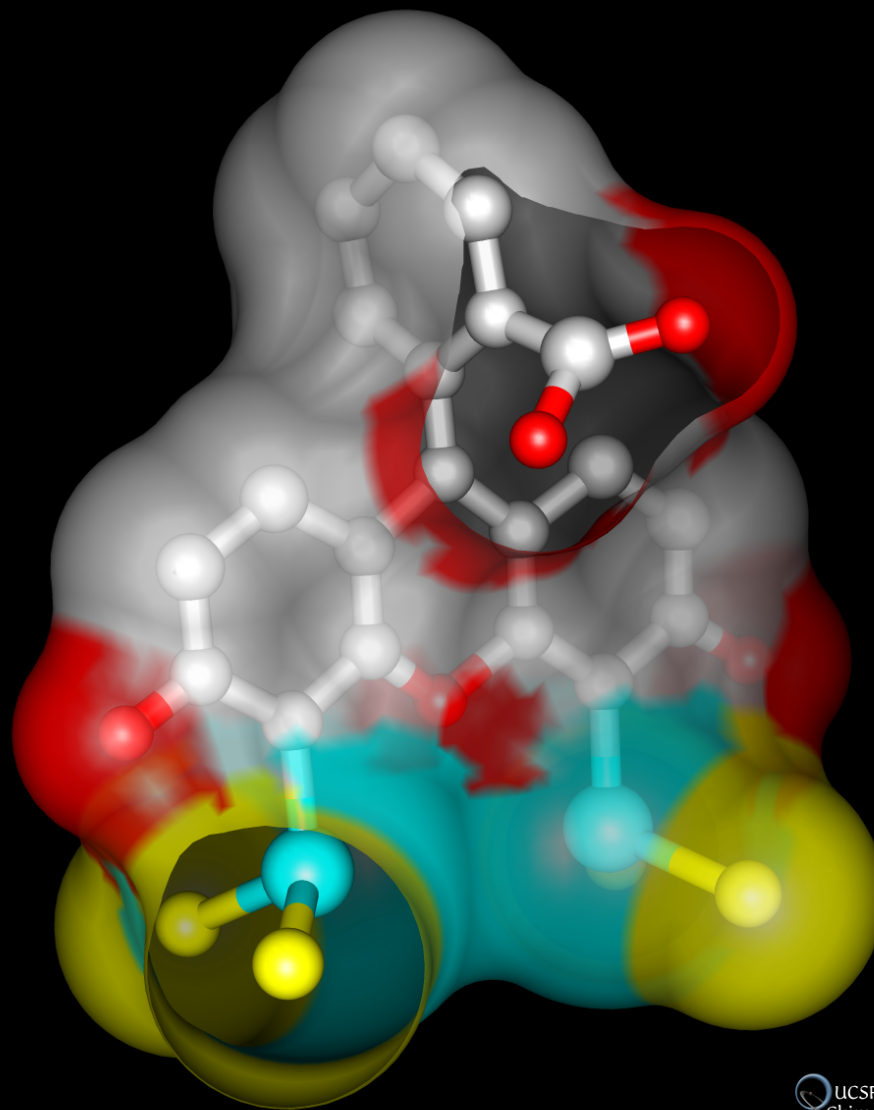


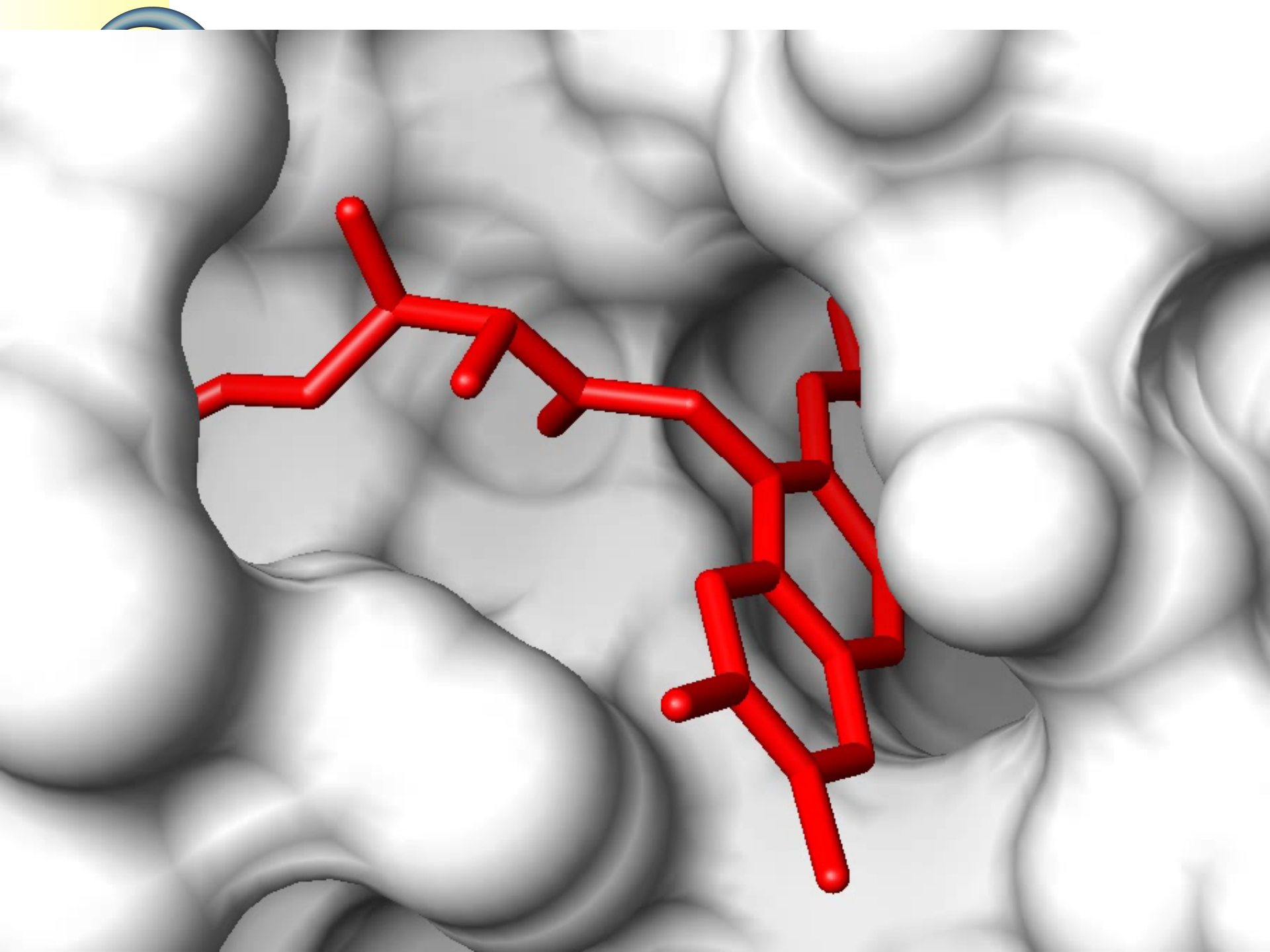


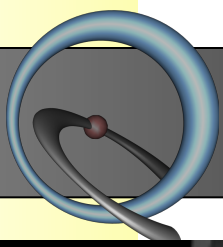


Other Visual Displays

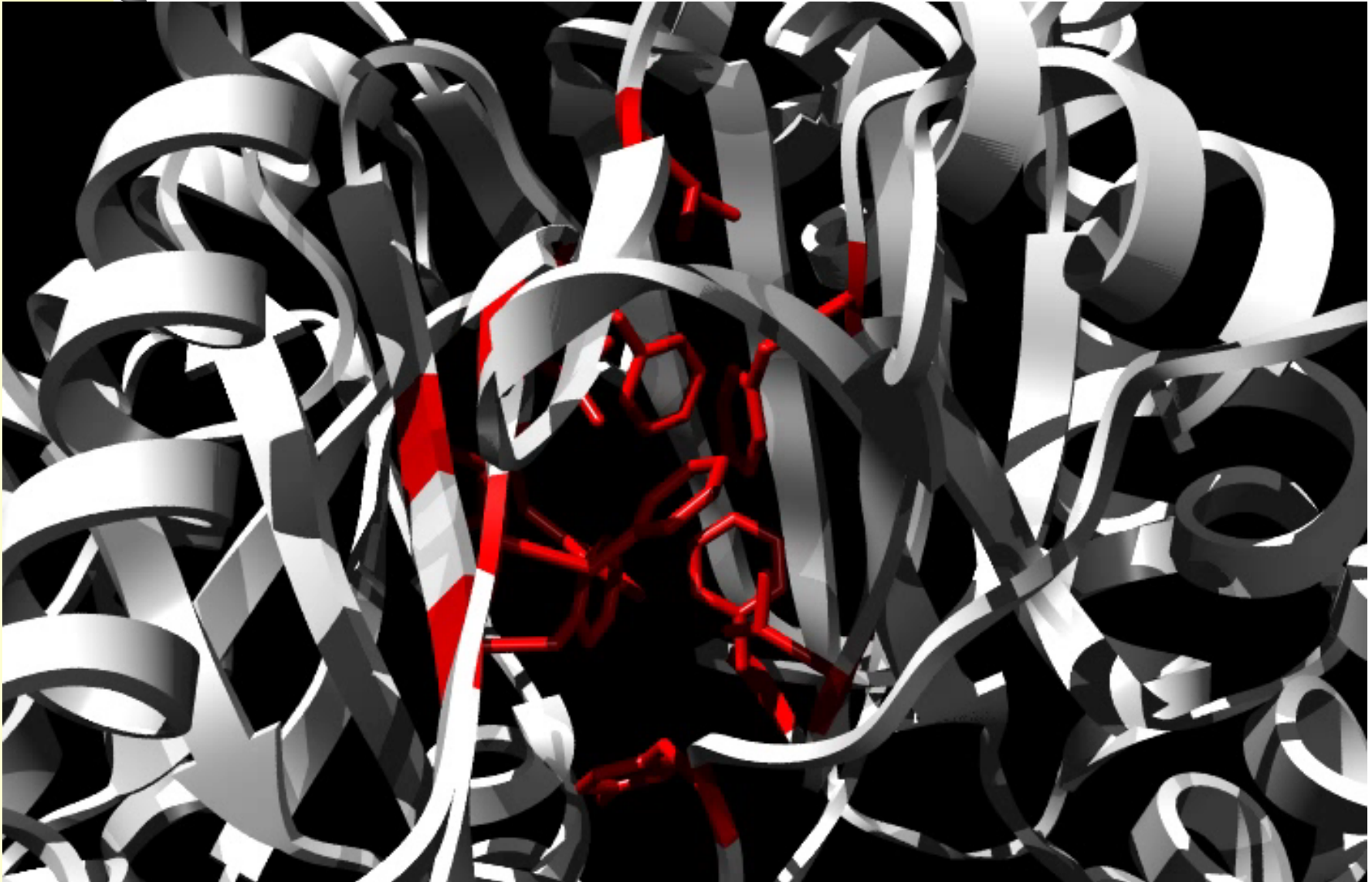
-
-
-
-
-
-

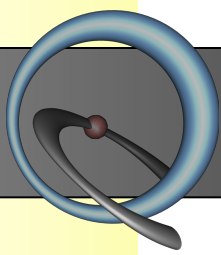






Animation





Animation

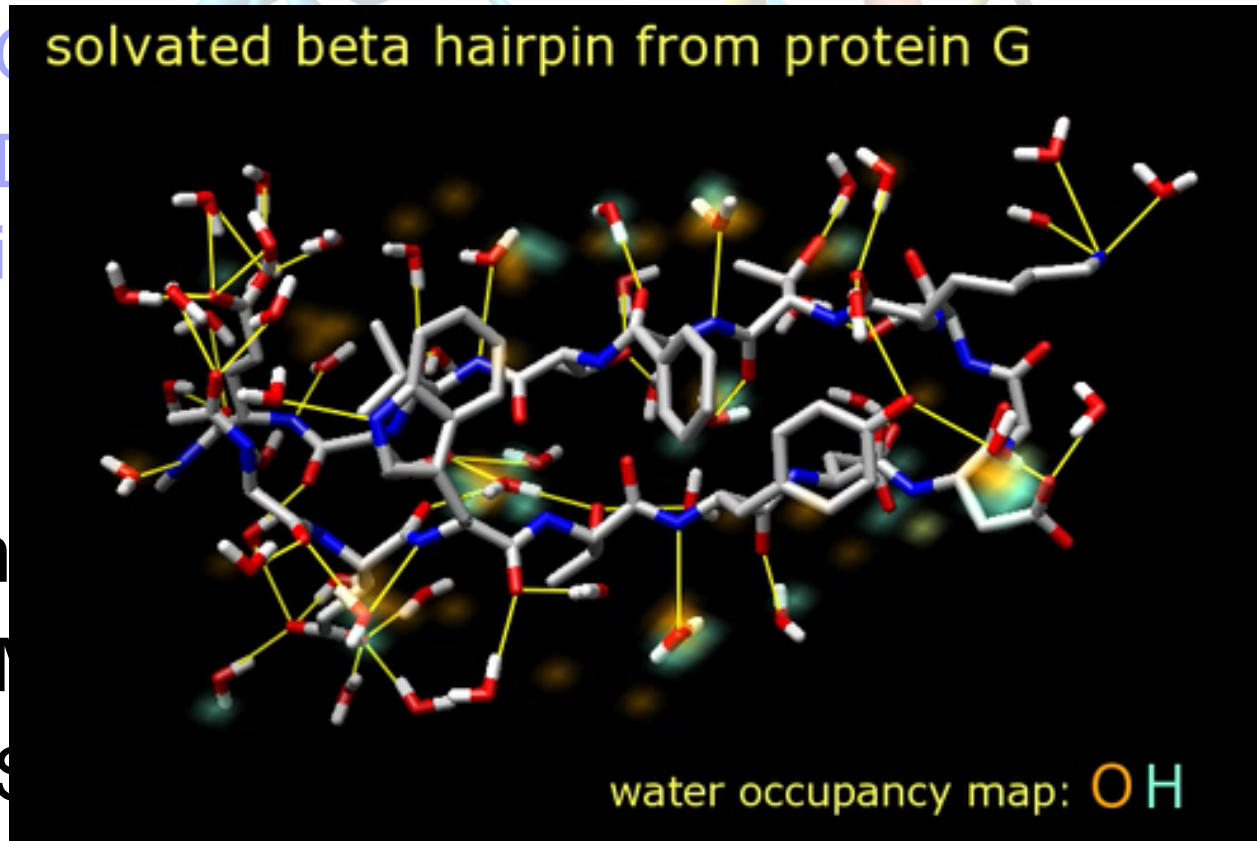
- Presentation

- (solvated beta hairpin from protein G) (ues)

- [unclear]

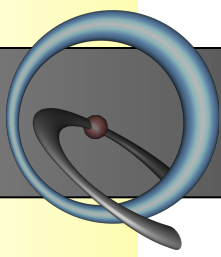
- Animation

- [unclear]
 - [unclear]



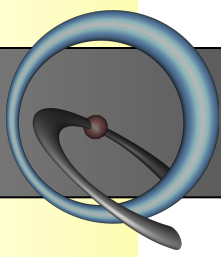
Animations





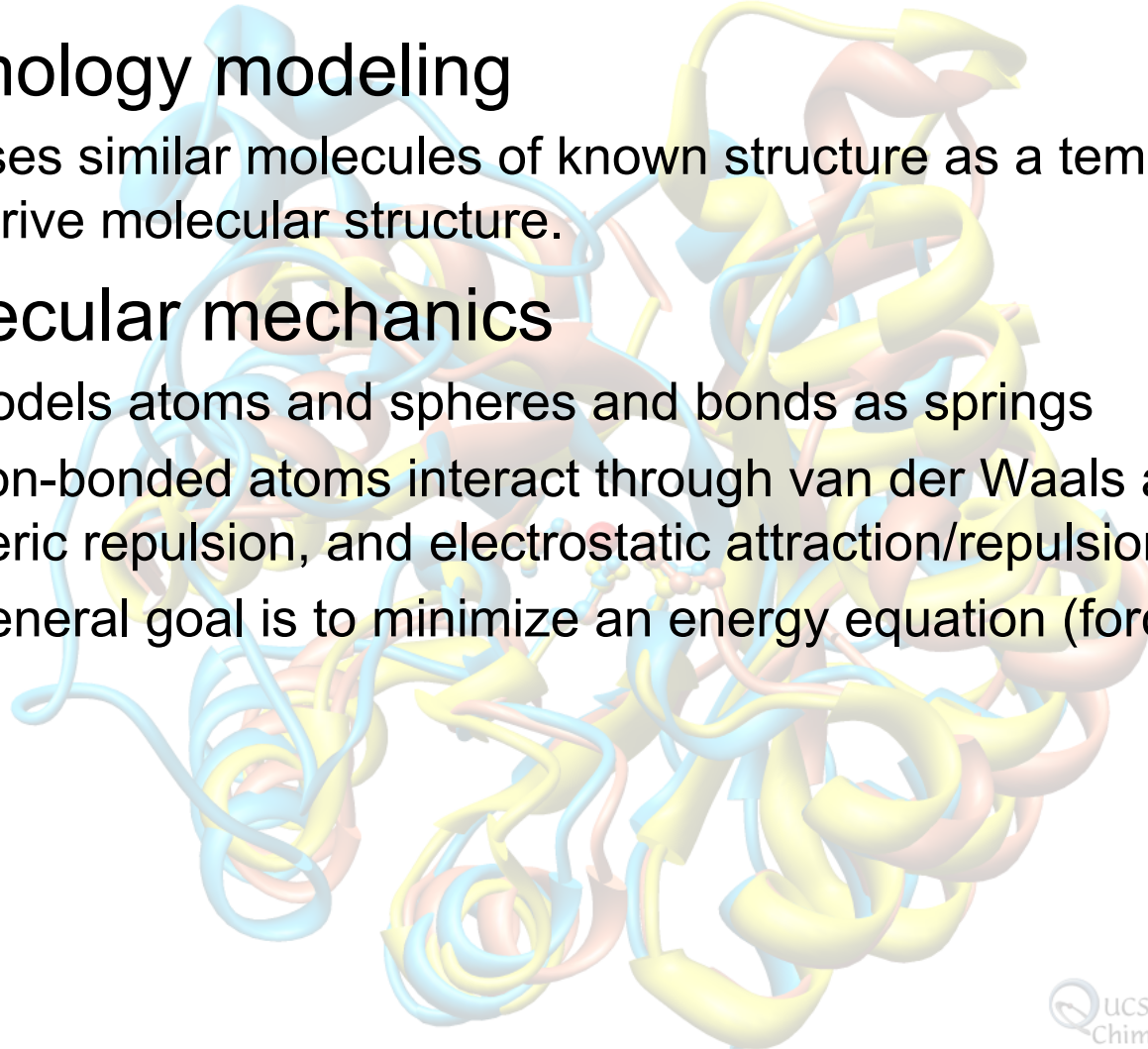
Manipulations

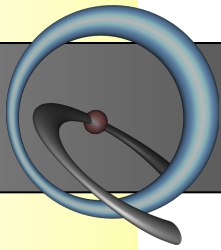
- Selection
- Movement
- Focus
- Zoom
- Changing representations
- Labeling
- Alignment
- Modeling “lite”
 - Bond adjustments
 - Adding/deleting/changing residues



Modeling

- **Homology modeling**
 - Uses similar molecules of known structure as a template to derive molecular structure.
- **Molecular mechanics**
 - Models atoms and spheres and bonds as springs
 - Non-bonded atoms interact through van der Waals attraction, steric repulsion, and electrostatic attraction/repulsion
 - General goal is to minimize an energy equation (force field)



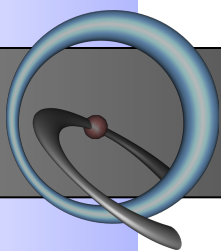


Modeling

- **Molecular dynamics**
 - Models the motions of a molecular system, including conformational transitions and local vibrations, using molecular mechanics force fields
 - Takes into account the thermodynamic environment
 - May be used to compute both thermodynamic and kinetic properties
 - Result is an ensemble (i.e., a movie) of how the molecule moves
- **Quantum (*ab initio*) modeling**
 - Structures are solved by approximating the Schrödinger equation for all particles (nuclei and electrons) in the system.

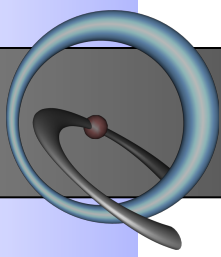
(see <http://cmm.info.nih.gov>)





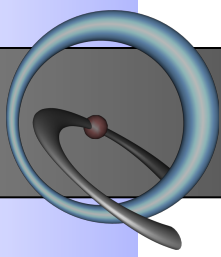
Applications of molecular visualization

- **Computational chemistry**
 - Dynamic molecules
 - Molecular interactions
- **Microscopy**
 - Lower resolution, volumetric data
- **Genomics**
 - Sequence-structure-function relationships
- **Systems biology**
 - Broad view across variety of data



Scenarios of use

- **Analysis**
 - Molecular dynamics
 - Docking
 - Sequence-structure relationships
 - Low-resolution representations
 - Viruses and large complexes
 - Electron microscopy
 - Structures in context
- **Publication**
 - High-resolution images
 - Animation



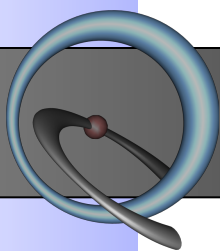
Molecular dynamics

The screenshot displays the UCSF Chimera software interface. The main window shows a protein structure with a grey electron density map. Below the main window are three panels:

- 1.2-1.4 RMSD Map:** Shows a heatmap of RMSD values. The x and y axes represent different frames or residues. The color scale ranges from black (low RMSD) to white (high RMSD).
- MD Movie: md01.crd:** Shows playback controls for the molecular dynamics simulation. It includes buttons for play, stop, and frame navigation. The current frame is 28 of 100, and the step size is 1. The playback speed is set to "slower".
- Volume Viewer:** Shows a histogram of density values. The range is 0 - 66, and the level is 16. The color is set to grey.

The status bar at the bottom of the main window indicates "366 atoms, 366 bonds".

Chimera



Docking

UCSF Chimera

ViewDock - H:\CSB2006\Dock\vas.mol2

S	Number	Name	Energy score ▲	HBonds (all)	HBond Ligand Atoms	HBond f
V	1	test_22	-42.64	8	5	1
V	2	test_27	-29.5	1	1	1
V	3	test_10	-28.4	0	0	0
V	4	test_19	-27.91	3	2	2
V	5	test_28	-26.87	1	1	1
V	6	test_04	-25.38	1	1	1
V	7	test_21	-22.99	1	1	1
V	8	test_07	-22.67	1	1	1
V	9	test_26	-22.59	0	0	0
V	10	test_16	-22.54	4	4	4
V	11	test_20	-22.35	2	2	2
V	12	test_17	-22.17	5	3	3
V	13	test_11	-19.81	3	3	3
V	14	test_15	-19.14	0	0	0

Chimera Model #2.1

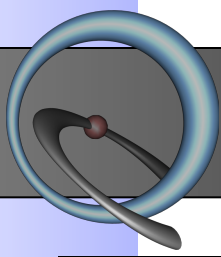
```
##### Number      : 1
##### Source num   : 22
##### Name         : test_22
##### Description  : ribose-monophosphate
##### Reflect      : 0
##### Energy score
:
-42.64
##### intermolecular van der Waals
-21.10
##### intermolecular electrostatic
-21.54
##### RMSD from input orientation (A)
```

Change Compound State

Viable Deleted Purged

no selection

Hide Quit Help



Sequence-structure relationships

The image shows two software windows. The left window, titled 'UCSF Chimera', displays a 3D ribbon model of a protein structure with magenta and grey ribbons. The right window, titled 'super8.msf', shows a sequence alignment of several protein sequences. The alignment is color-coded by amino acid type and includes a conservation plot above the sequences. The 'enolyeast' sequence is highlighted in pink in both the alignment and the Chimera window.

gald	...	V	S	A	P	MAK	V	L	I	K	E	L	E							
mleiipp	...	W	D	E	S	Q	A	I	R	A	C	Q	V	L	G					
mleiipp	...	W	D	E	N	T	A	S	V	W	I	P	R	L	E					
naaar	...	Y	T	L	G	D	A	P	Q	.	L	A	R	L	D					
maalct	A	D	Y	I	Q	T	L	A	E	A	A					
enolyeast	D	K	S	K	W	L	T	G	P	Q	L	A	D	L	Y	H	S	L	M	K
enolhal	S	T	E	E	.	.	I	E	Y	I	A	G	K	V	E	.

141
Consensus pygllliEqP
Conservation
mr QEGVTWIEEP TLQHD...Y
gald PYRPLFIEEP VLAEQ...A
mleiipp DNGIDLIEQP ISRIN...R
mleiipp AAGVELVEQP VARSN...F
naaar PFGLLLIEQP LEEED...V
maalct PFHLR.IEGP MDVEDRQKQM
enolyeast RYP.IVSIEDP FAEDDWEAWS
enolhal EYDLVYVEDP LDENDYEAF A

161
Consensus eghar laaql
Conservation
mr EGHQR IQSKL NVP...VQM
gald EYYPKLA AQT HIP...LAA
mleiipp GGQVRLNQRS PAP...IMA
mleiipp DALRRLSADN GVA...ILA
naaar LGHAELARRI QTP...ICL
maalct EAMRDLRAEL DGRGVDAELV
enolyeast HFFKTAGIQ .IVA...
enolhal DLTAQVGDQT LVCG...
181
Consensus .de.lfstnd
Conservation
mr GEN.WLGP EE MFKALSI...

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Command: repr sphere

Active models: 0 1 2 3 4 5 6 7 8 9 All

no select

Volume Viewer

File Features

Data emd_1283.map Size (120,120,120) Step 1 1 1

Show surface mesh solid

Ctrl-click on histogram to add or delete thresholds

Range -0.159 - 0.587 Level 0.311 Color

- Surface smoothing iterations 2 factor 0.5
- Subdivide surface 1 times
- Smooth mesh lines
- Square mesh
- Mesh line thickness 1 pixels
- Dim transparent surface/mesh
- Mesh lighting
- Two-sided surface lighting
- Light flip side for thresholds < 0

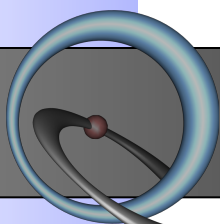
Show Unshow Center Orient Close Help

Viewing

Camera Side View Rotation Effects Lighting

View All View: right Resolution: high

Reset Restore Save Close Help



Multiscale representations

UCSF Chimera

File Select Actions Presets Tools Favorites Help

IDLE

View Dock

Command:

Active models: 0 1 2 3 4 5 6 7 8 9 All

up-arrow to increase selection (atoms->residues->chains etc.) no selecti

Multiscale Models

Select chains

All With loaded atoms Clear

Extend Up Copies Atoms Loaded atoms

Near Contacts Range 5 Load atoms

Act on selected chains

Selected chains Show Hide Hide all styles

Other chains Show Hide Hide all styles

Style Show... Show also... Hide...

Color Transparency 0

Color Atoms Ribbons to match surfaces

Resurface Resolution 8

Delete chains

Models from molecules and matrices

Multimer: Biological oligomer (BIOMT)

Make models Delete selected models

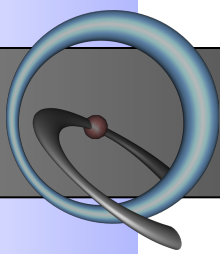
Close Help

Viewing

Camera Side View Rotation Effects Lighting

View All View: right Resolution: high

Reset Restore Save Close Help



Structures in context

Cytoscape Molecular Structure Navigator

Chimera View Select

- 10 Open Chimera Models
 - Node gi129176 [Model #0 1QW7 (1 chains, 336 re
 - Node gi14719485 [Model #1 1JGM (1 chains, 335
 - Node gi2392286 [Model #2 1DPM (1 chains, 329 r
 - Node gi2098312 [Model #3 1PSC (1 chains, 329 r
 - Node gi5542102 [Model #5 1BF6 (1 chains, 291 r
 - Node gi12084365 [Model #6 1EYW (1 chains, 332
 - Node gi12084365 [Model #7 1E2Z (2 chains, 333
 - Chain A (331 residues)
 - Chain het (2 residues)
 - DII 1403
 - DII 2403
 - Node gi13786719 [Model #8 1I0B (1 chains, 334
 - Node gi13786719 [Model #9 1HZY (1 chains, 334
 - Node gi13786719 [Model #10 1I0D (1 chains, 334

Reference Structure

Node gi12084365; model 1E2Z

Match Stru...	Aligned Pairs	RMSD	Score
1BF6	214	0.992	491.5
1PTA	253	0.86	1,493.4
1I0B	329	0.225	1,663
1JGM	329	0.233	1,670.2
1DPM	329	0.135	1,671.8

Show sequence panel for each alignment
 Assign results to Cytoscape edge attributes

Done Align

Cytoscape Desktop (Session: pte.cys)

SFLD Search: []

Amidohydrolase Superfamily--child

CytoPanel 2

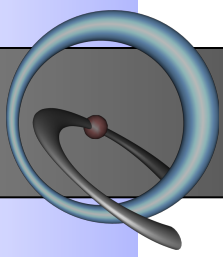
ID	subgroup	FunctionalResidues
gi15212234	phosphotriesterase like	
gi12084365	phosphotriesterase like	His55,His57,Lys16...
gi129176	phosphotriesterase like	
gi13786719	phosphotriesterase like	His55,His57,Lys16...
gi2392286	phosphotriesterase like	His55,His57,Lys16...
gi2098312	phosphotriesterase like	His55,His57,Lys16...
gi14719485	phosphotriesterase like	His55,His57,Lys16...

Node Attribute Browser Edge Attribute Browser Network A

Right-click + drag to ZOOM Middle-click + drag to PA

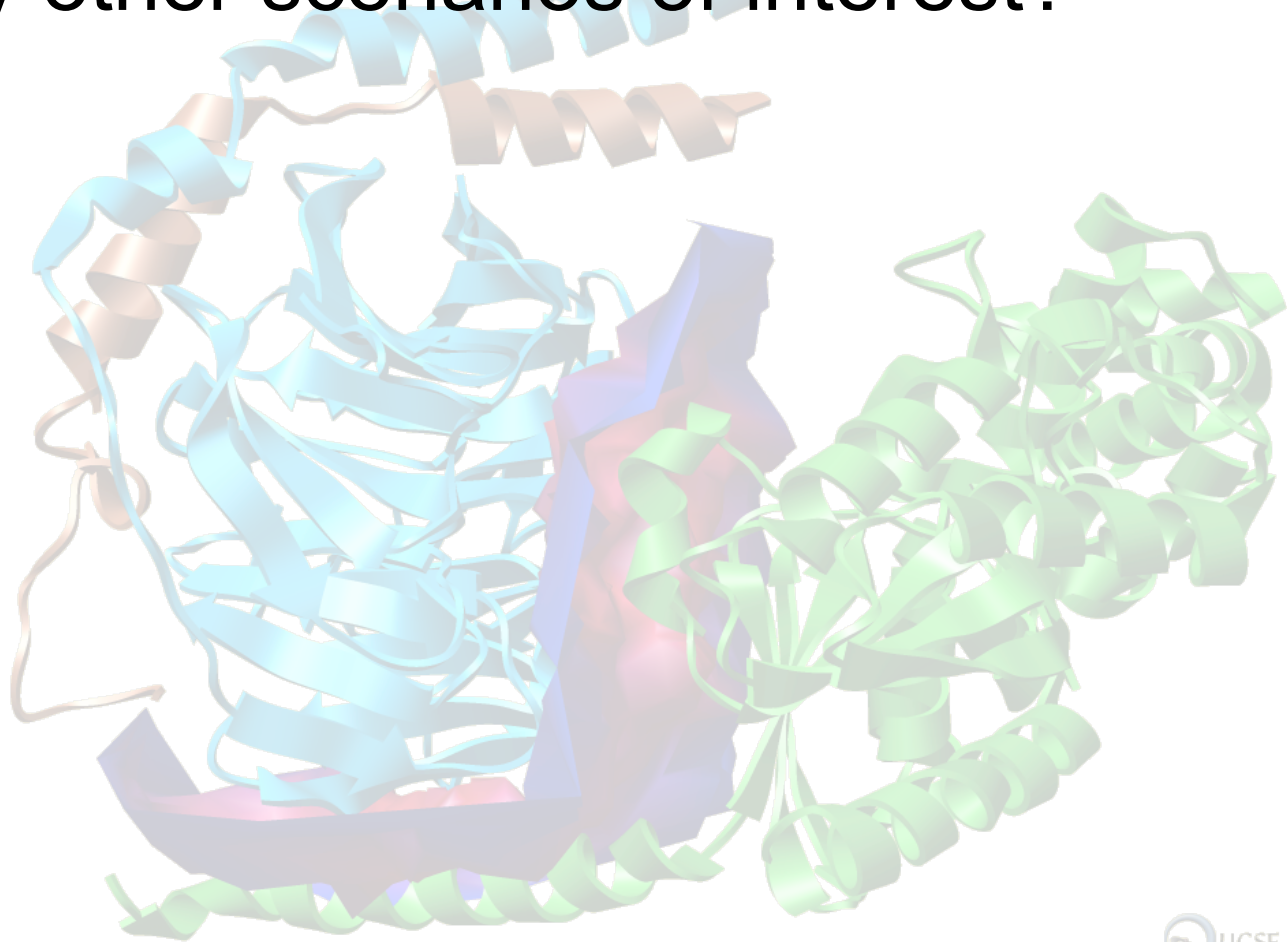
UCSF Chimera

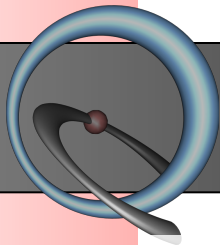
File Select Actions Tools Favorites Help



Questions?

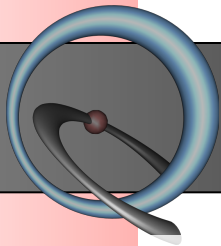
- Any other scenarios of interest?





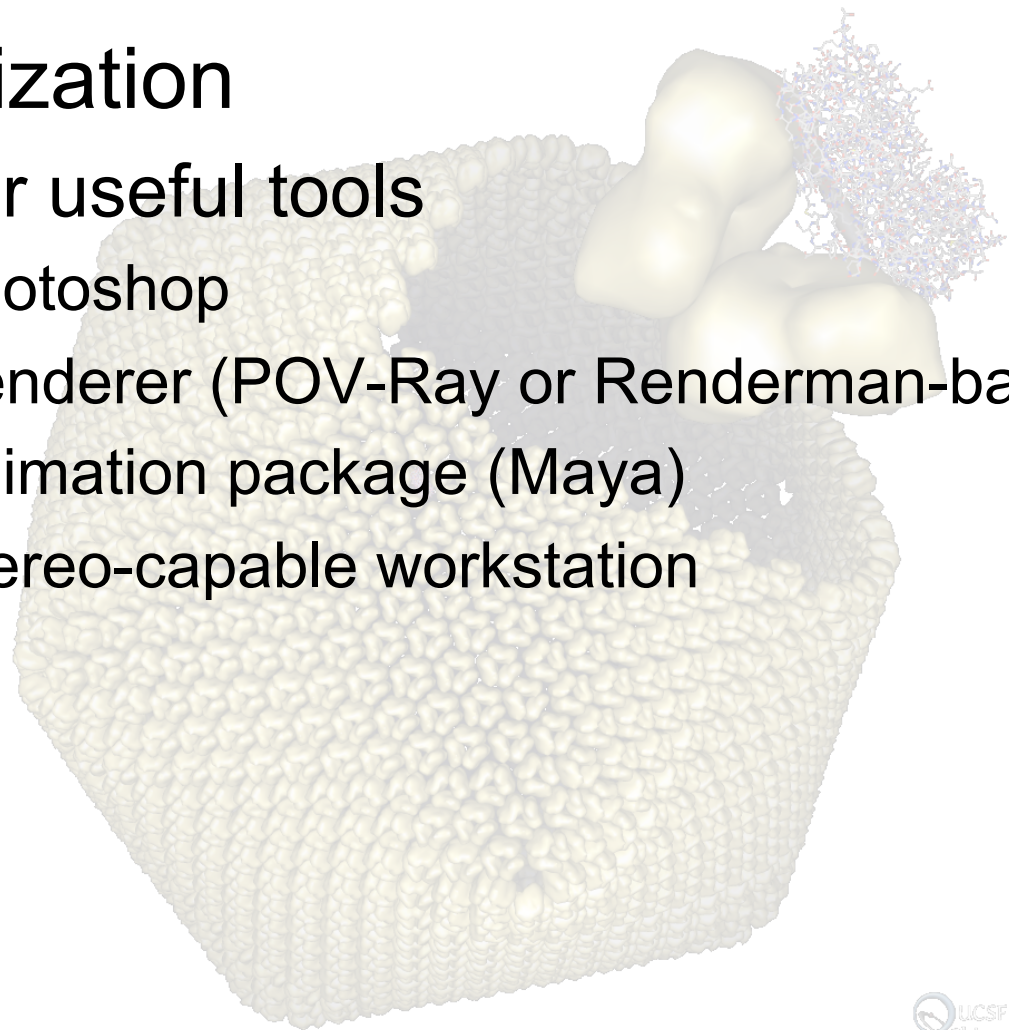
Available Tools

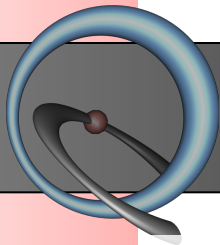
- Visualization
 - “Full featured” academic packages
 - UCSF Chimera (<http://chimera.ucsf.edu/>)
 - PyMOL (<http://pymol.sourceforge.net/>)
 - VMD (<http://www.ks.uiuc.edu/Research/vmd/>)
 - Viewers
 - Jmol (<http://jmol.sourceforge.net/>)
 - RasMol/Chime (<http://www.openrasmol.org/>)
 - SwissProt PDB-Viewer (DeepView) (<http://www.expasy.org/spdbv/>)
 - RCSB Protein Workshop (<http://www.rcsb.org/>)



Available Tools

- Visualization
 - Other useful tools
 - Photoshop
 - Renderer (POV-Ray or Renderman-based)
 - Animation package (Maya)
 - Stereo-capable workstation

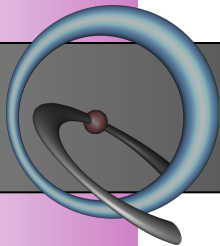




Available Tools

- Analytical tools (partial list)
 - PROCHECK (<http://www.biochem.ucl.ac.uk/~roman/procheck/>)
 - Structure-Function Linkage Database (<http://sfld.rbvi.ucsf.edu/>)
 - ExPASy (<http://www.expasy.org/>)
- Modeling tools
 - Amber (<http://amber.scripps.edu/>)
 - Charmm (<http://www.charmm.org/>)
 - NAMD (<http://www.ks.uiuc.edu/Research/namd/>)
 - Gaussian (<http://www.gaussian.com/>)
 - ModBase (<http://modbase.compbio.ucsf.edu/>)
 - Modeller (<http://www.salilab.org/modeller/>)
 - DOCK (<http://dock.compbio.ucsf.edu/>)
 - Many, many more (see <http://cmm.info.nih.gov/>)





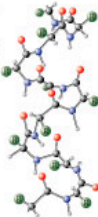
Comparison of Visualization Packages

Jmol Protein Secondary Structure


UCSF Chimera

Alpha-helix

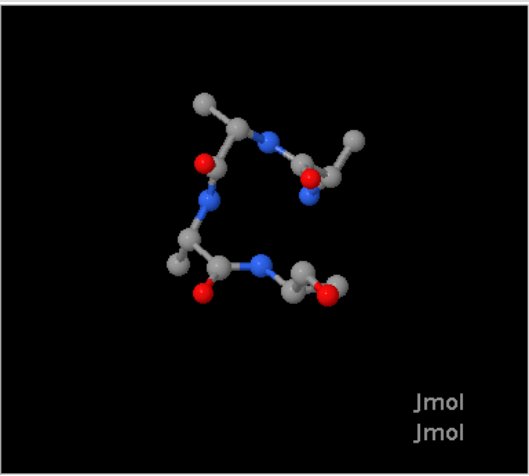
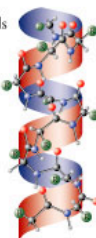
Ball-and-stick model of a portion of the α -helical secondary structure of a protein molecule



This ribbon model shows the general arrangement of atoms in a portion of the α -helical secondary structure of a protein molecule.

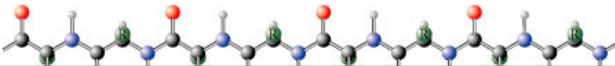


The two models superimposed



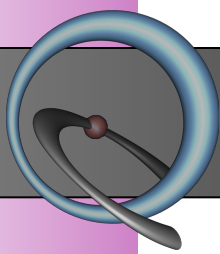
Jmol
Jmol

Beta-Sheet



Jmol script completed

Adblock



Comparison of Visualization Packages

Grab File Edit Capture Window Help Thu 7:43 PM

PyMOL Viewer

(all) [S] [H] [L] [C]
 ref [S] [H] [L] [C]
 2fofc [S] [H] [L] [C]
 m1 [S] [H] [L] [C]
 dist01 [S] [H] [L] [C]
 dist02 [S] [H] [L] [C]
 dist03 [S] [H] [L] [C]
 dist04 [S] [H] [L] [C]
 dist05 [S] [H] [L] [C]
 dist06 [S] [H] [L] [C]
 dist07 [S] [H] [L] [C]
 dist08 [S] [H] [L] [C]
 dist09 [S] [H] [L] [C]
 dist10 [S] [H] [L] [C]
 dist11 [S] [H] [L] [C]
 dist12 [S] [H] [L] [C]
 dist13 [S] [H] [L] [C]
 dist14 [S] [H] [L] [C]
 dist15 [S] [H] [L] [C]
 dist16 [S] [H] [L] [C]
 dist17 [S] [H] [L] [C]
 dist18 [S] [H] [L] [C]
 dist19 [S] [H] [L] [C]
 dist20 [S] [H] [L] [C]
 dist21 [S] [H] [L] [C]
 dist22 [S] [H] [L] [C]
 dist23 [S] [H] [L] [C]

Mouse: L M R
 None Rota Move MovZ
 Shift RotZ Move Clip
 Ctrl +lb PKAt PKBd
 CtSh lb Orig rb

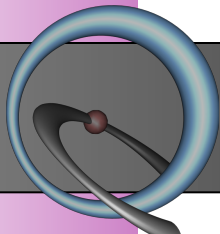
Frame| 1/ 1| 4/s

```

PyMOL>11.614999771, 30.190002441, 20.704999924,\
PyMOL>27.582914352, 35.903400051, 1.000000000 )
Scene: view updated.PyMOL>set nonbonded_size=0.6
Setting: nonbonded_size set to 0.60000.
ObjectMesh: updating "m1".
IsosurfVolume: Surface generated using 16155 lines.
  
```

PyMOL>

Macintosh HD
 Desktop (Mac OS 9)
 pymol-0_59.tgz



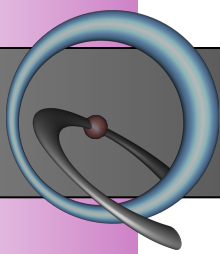
Comparison of Visualization Packages

The screenshot displays the vmd OpenGL Display interface. The central window shows a protein structure with a purple ribbon and a blue ribbon, with a red and white stick model in the center. The interface includes several panels:

- molWi**: Draw Molecule panel with checkboxes for m1, m2, and NOE.
- Main**: A menu with options like Main, Mol, Animate, Edit, Graphics, Labels, Render, Display, Color, Sim, Tracker, Help, and Quit.
- Mouse**: A panel with a 'Choose' dropdown and buttons for rotate, translate, scale, and pick.
- torsion**: A table for defining torsion restraints.
- Edit**: A panel for editing m2, including 'Detect collisions with' and 'Rotate'/'Translate' controls.
- NOE**: A panel for loading and selecting NOE restraints.
- Terminal**: A command window at the bottom showing the execution of commands like 'PS>vmd "noe load 0 1 noe.in"'.

DEL	side chain	ADD	RESET	?
0	PHE302:CHI1	f	-166.74	reset
1	PHE302:CHI2	f	89.98	reset

```
PS>
PS>vmd "noe load 0 1 noe.in"
2
PS>
```

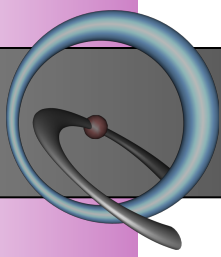


Comparison of Visualization Packages



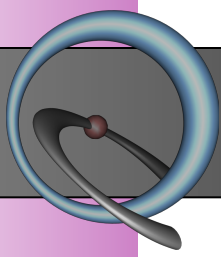
– Chimera

- best-in-class for visualizing very large structures
 - multiscale extension
 - volume viewer
- focus on extensibility, broad functionality
- primarily analytical interface
- familiar GUI interface (+command line)
- scriptable
- reasonable tools for publication & presentation
- embedded ray tracer (POV-Ray)
- excellent sequence/structure capabilities
- reasonable interface to modeling programs



Comparison of Visualization Packages

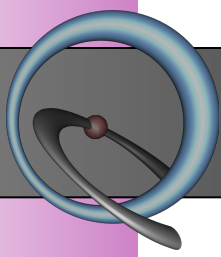
- Caveats
 - Our focus is primarily on Chimera
 - We are not users of other packages
 - There is no “best” package for everything (in our opinion)
 - YMMV (Your Mileage May Vary)
 - What we think is easy, you may think is hard
 - What we think is hard, you may think is easy
 - Choosing the best package for you
 - Does what you need
 - Good documentation
 - Good support (either local or from the authors)



UCSF Chimera

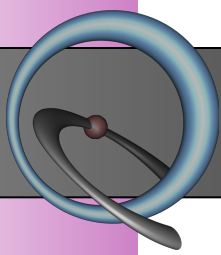


- Target audience
 - Scientists who need to analyze and model molecular systems in some detail
 - Scientists who want to develop new analytical methods
 - Scientists or educators who wish to communicate biological concepts visually
- Organization
 - Core features
 - Additional tools



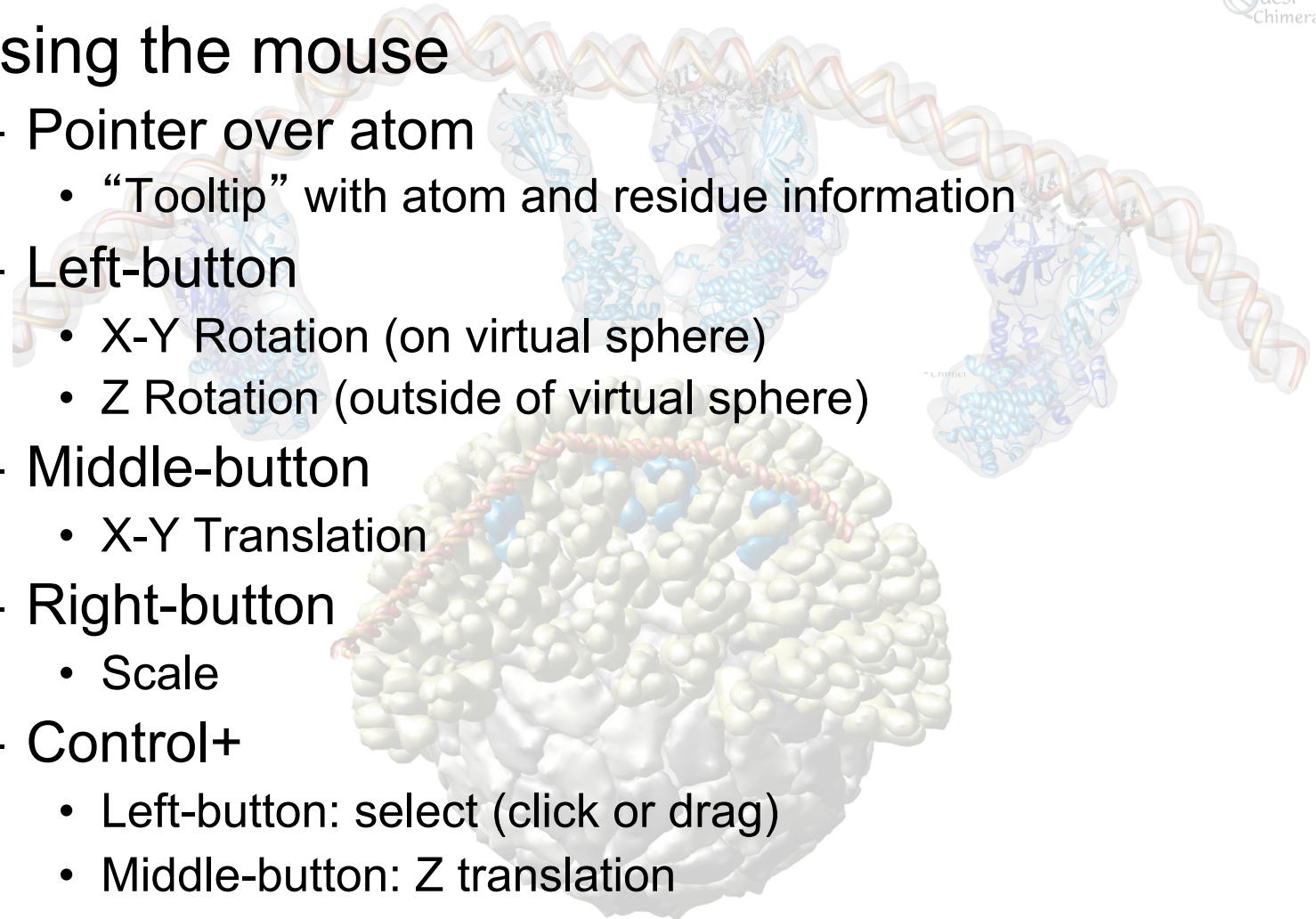
Chimera Core Features

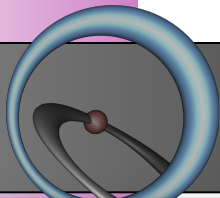
- Concepts
 - Graphical manipulation
 - Chemical knowledge
 - Hierarchy: Model→Chain→Residue→Atom
 - Attributes available at model, residue, and atom levels
 - Selection - Action
 - GUI/Command-line equivalence
 - For core, not necessarily extensions



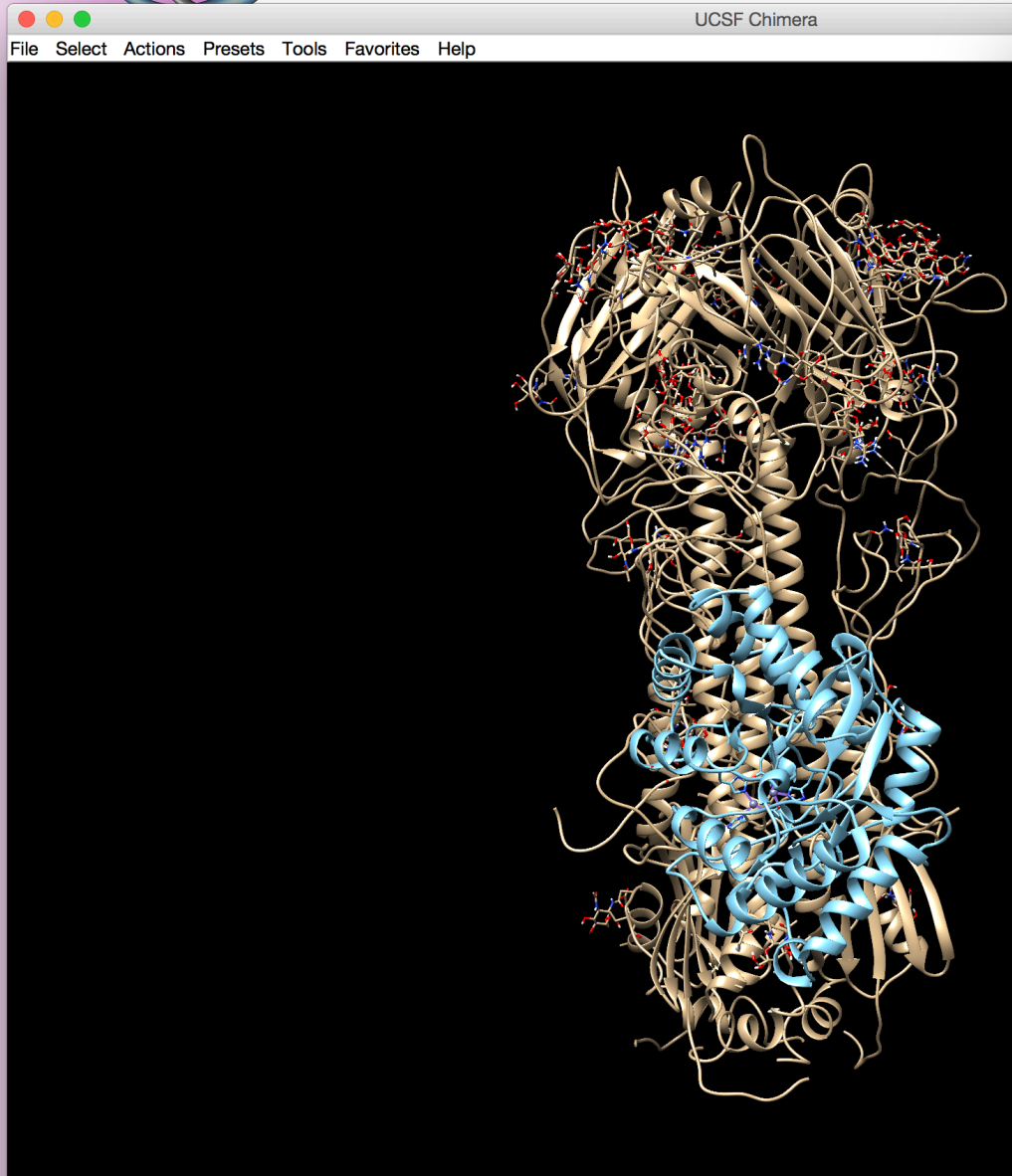
Core Features (cont.)

- 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.)



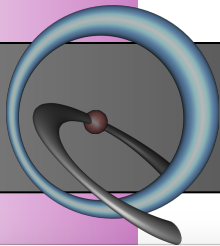
Viewing

Camera Side View Rotation Effects Lighting

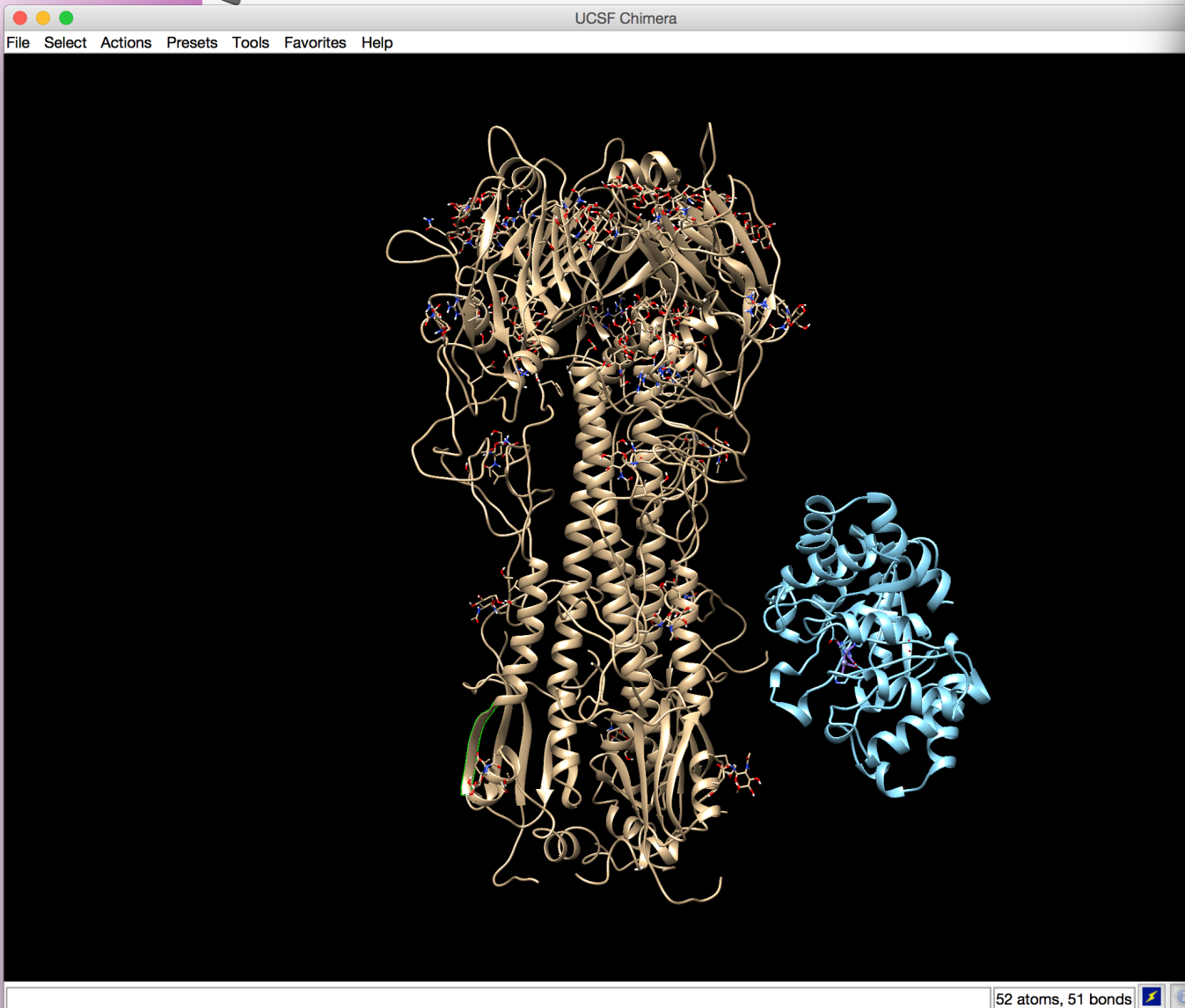
A diagram within the viewing panel showing a yellow square on the left representing the camera's field of view. Two red lines extend from the square to the right, forming a cone that encompasses a 3D protein model. Two vertical yellow lines are positioned on either side of the protein model, likely representing clipping planes.

Clip Surface capping... View All Side: right

Reset Restore Save Close Help



Core Features (cont)



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: [dropdown]

aromatic ring style: disk

auto-chaining: on

ball scale: 0.25

color: [color swatch]

displayed: true

line style: [dropdown]

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

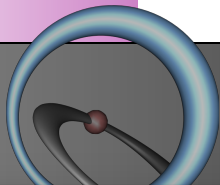
surface color: No

surface opacity: -1.0

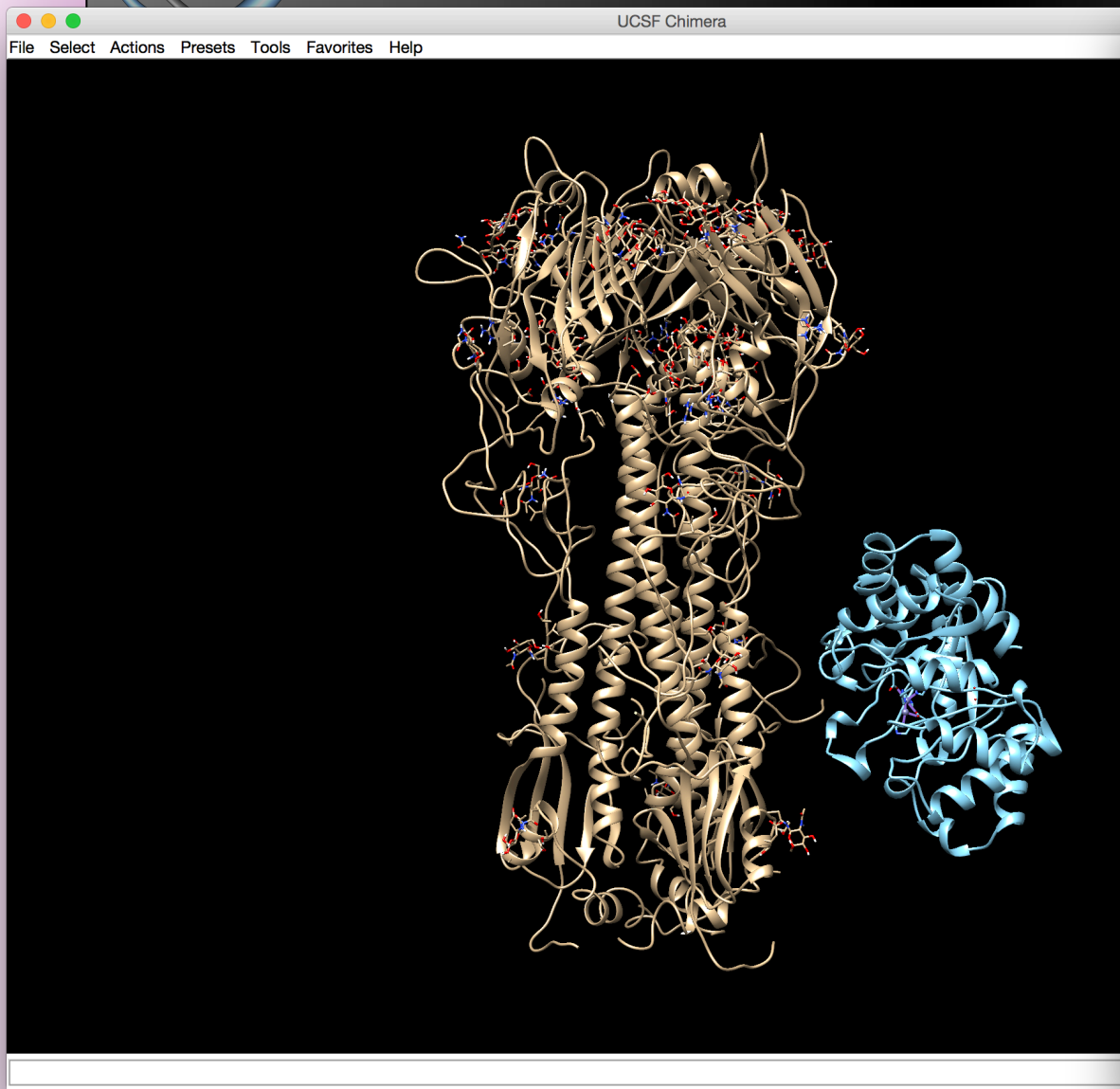
vdw density: 5.0

vdw dot size: 1.0

Write List... Write PDB... Close Help



Core Features (cont.)



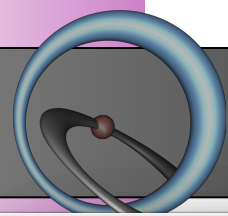
Model Panel

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



Core Features (cont.)

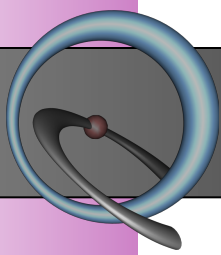
MultiAlignViewer

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 - -
	51	61	71	81	91
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
	101	111	121	131	141
Consensus	f l n R S i d E i A	d l f i h d i k e G	I q G T l 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 g	I T k d v E K V i r

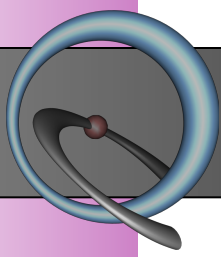
Alignment reformatted

Quit Hide Help



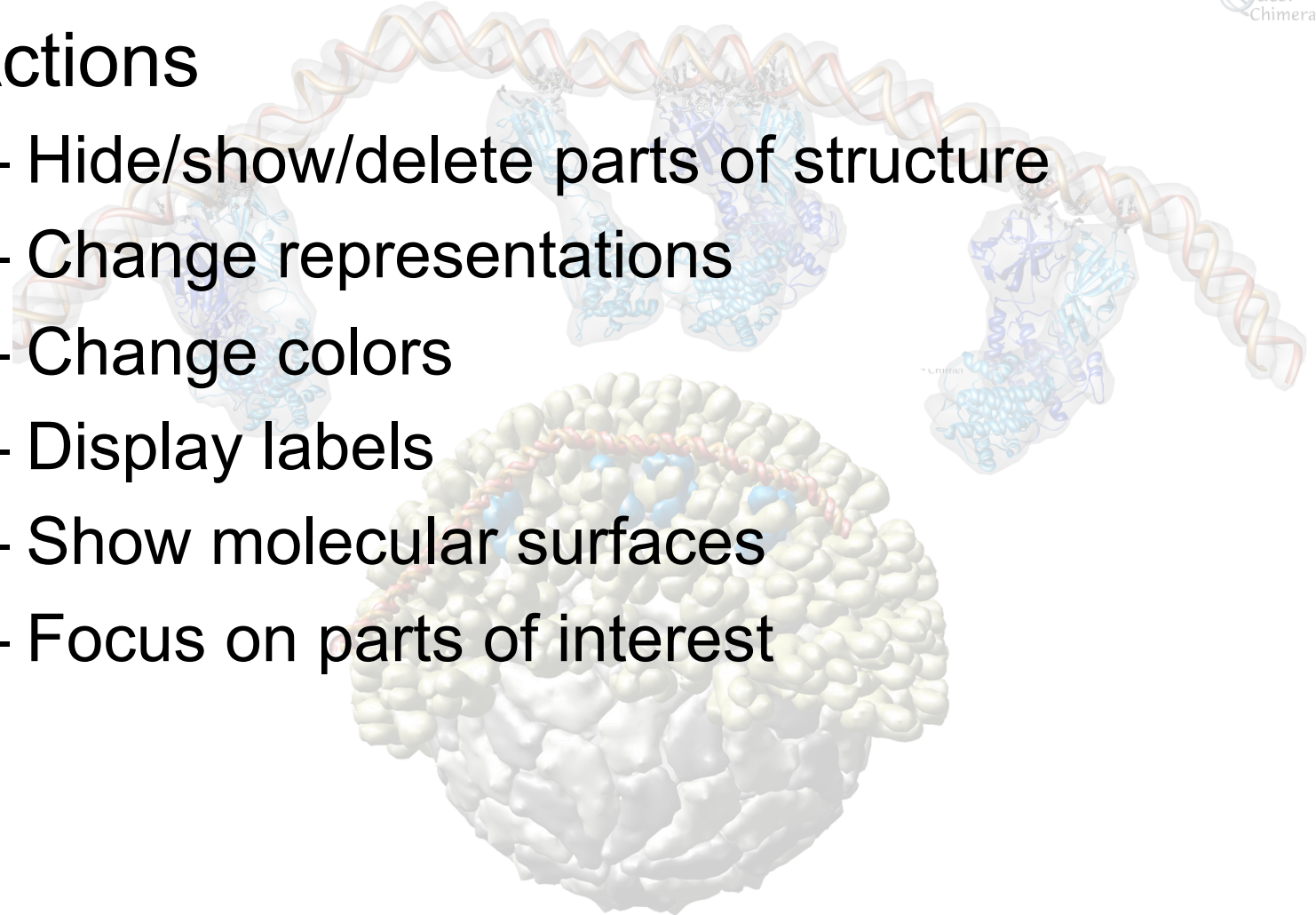
Core Features (cont.)

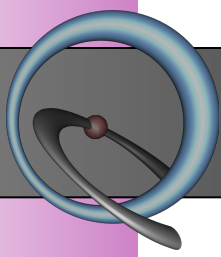
- Selection methods
 - Using mouse
 - Control-click and control-drag
 - Shift-control-click and shift-control-drag to add to selection
 - By atom and residue names and types
 - By higher order structure
 - e.g., chains, ligands, solvent
 - By spatial location
 - e.g., within some distance of another 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.)

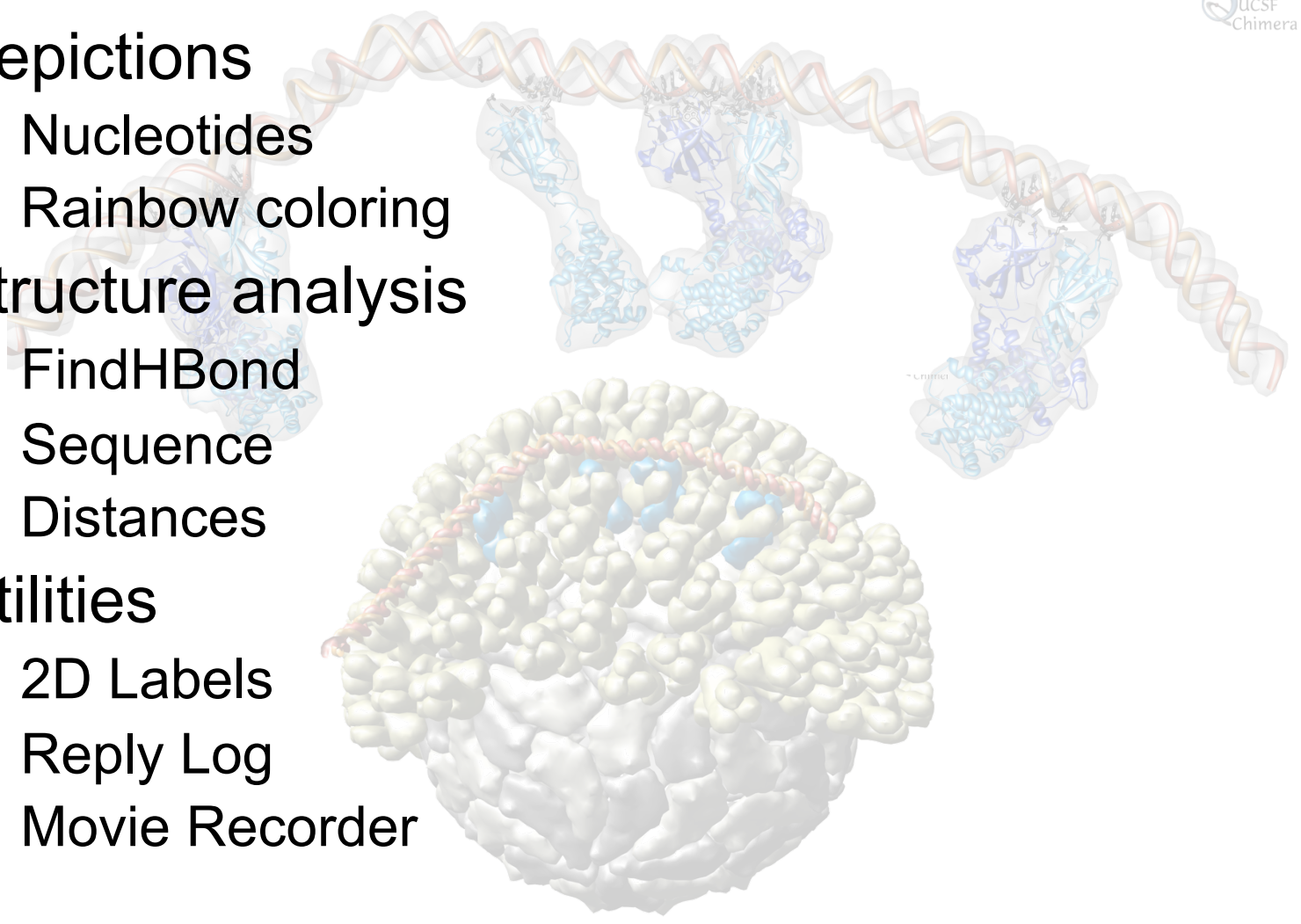
- **Actions**
 - Hide/show/delete parts of structure
 - Change representations
 - Change colors
 - Display labels
 - Show molecular surfaces
 - Focus on parts of interest

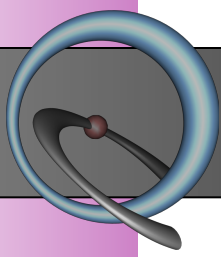




Commonly used tools

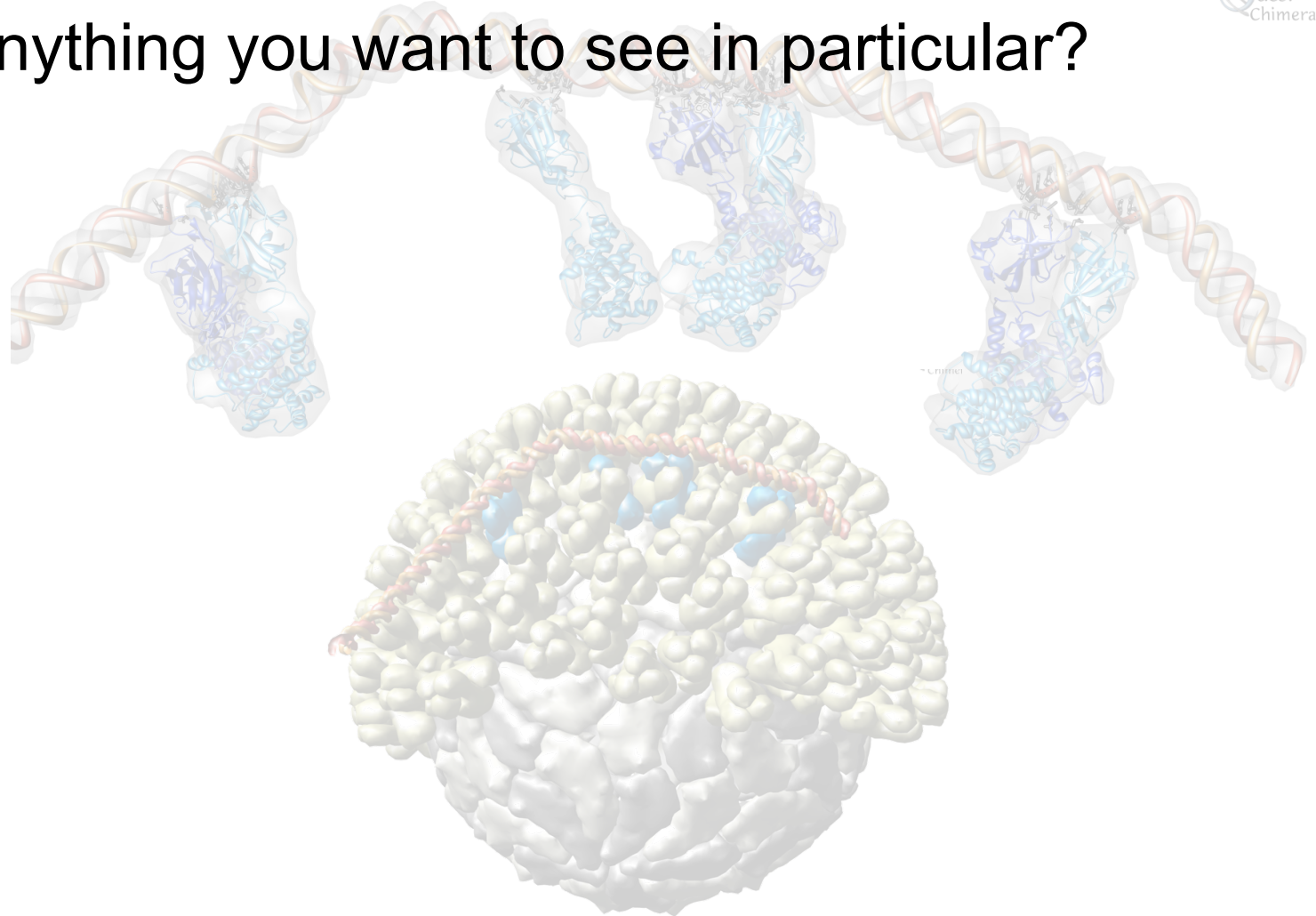
- Depictions
 - Nucleotides
 - Rainbow coloring
- Structure analysis
 - FindHBond
 - Sequence
 - Distances
- Utilities
 - 2D Labels
 - Reply Log
 - Movie Recorder

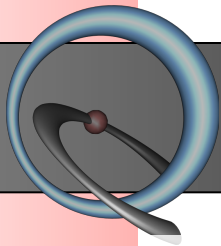




Questions?

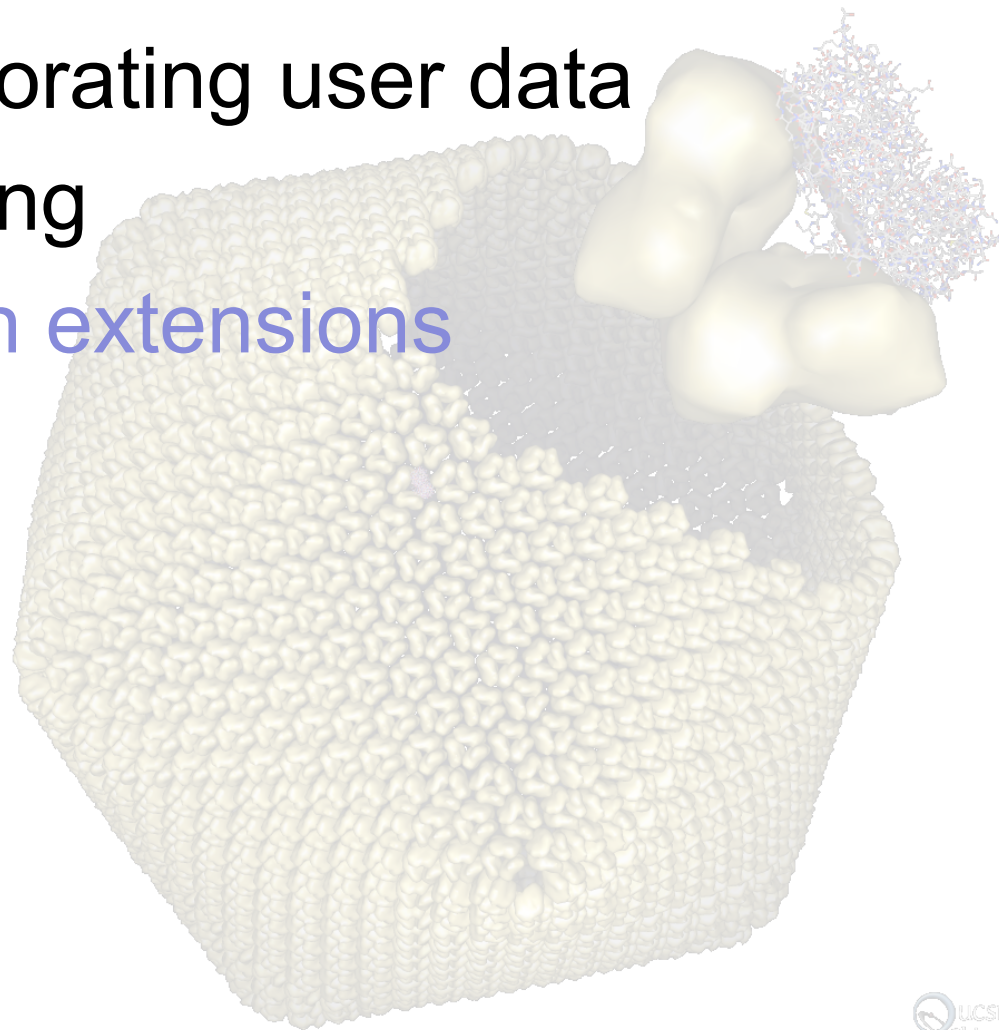
- Anything you want to see in particular?

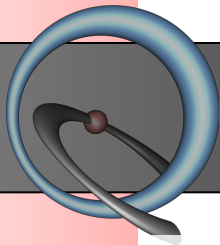




Extending Chimera

- Incorporating user data
- Scripting
- Python extensions



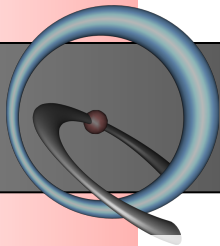


Incorporating user data

The screenshot displays the UCSF Chimera interface. The main window shows a 3D molecular model with atoms in grey and bonds in white. Some atoms and bonds are highlighted in green and magenta. The status bar at the bottom indicates "231 atoms, 227 bonds".

Two dialog boxes are open on the right side:

- Render/Select by Attribute:** This dialog is used to select and render atoms based on a specific attribute. It shows the "Attributes of" dropdown set to "residues" and the "Models" list containing "3fx2.pdb (#0)". The "Attribute" is set to "mw". A histogram shows the distribution of molecular weights, with a value of 192.585 selected. The "Select" options are "between markers (inclusive)" and "outside markers".
- Attribute Calculator:** This dialog is used to calculate a new attribute for the selected residues. The "Calculate attribute" is set to "mw" for "residues". The formula entered is "sum(atom.aw)". The "Restrict attribute assignment to current selection, if any" checkbox is checked. The "Open Render/Select by Attribute" checkbox is also checked.



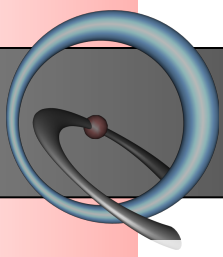
Scripting

The screenshot displays the UCSF Chimera interface. The main window shows a 3D model of a protein structure with a red ribbon highlighting a specific region. The status bar at the bottom indicates "no selection".

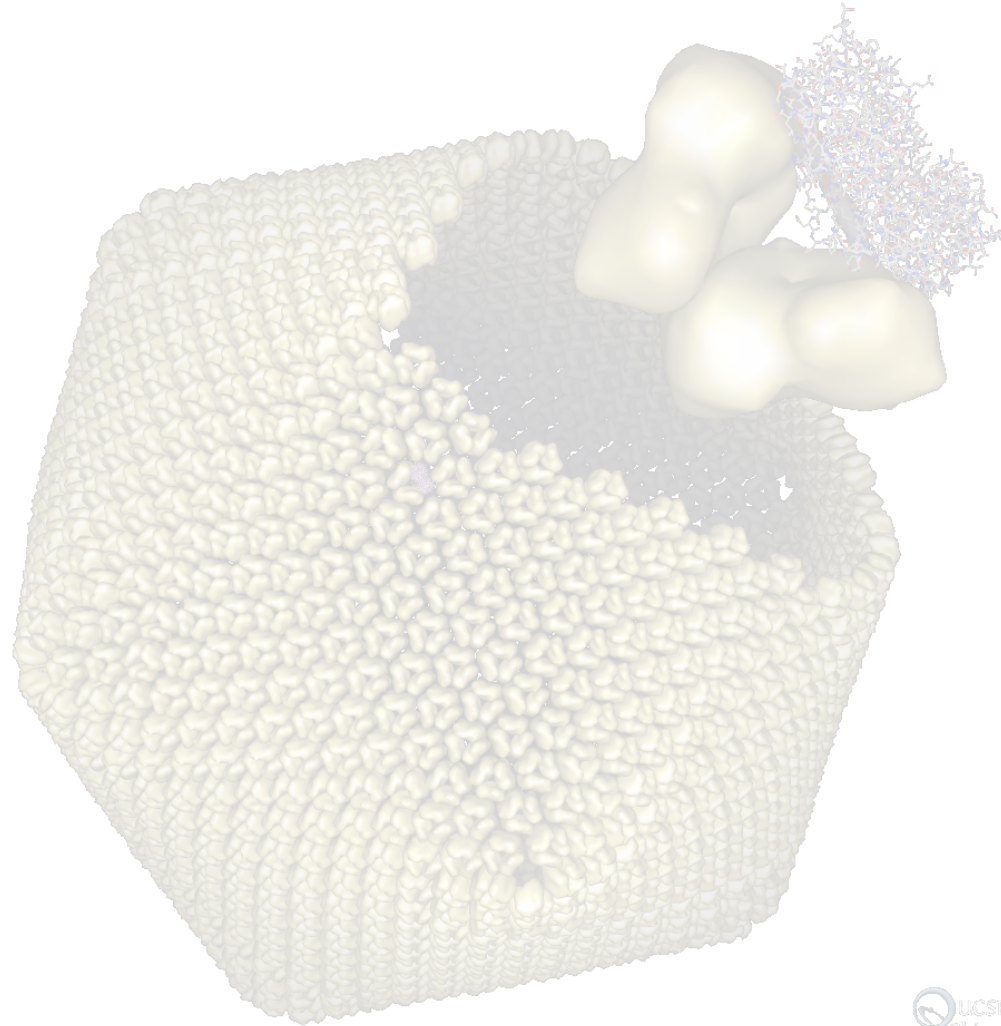
On the right side, there are two panels:

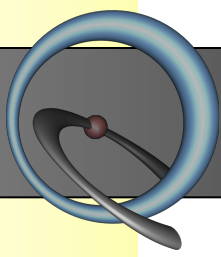
- Demo Editor - Silly Demo [H:\CSB2006\defattr\silly.src]**: This panel contains a list of panels on the left, with "Rotations" selected. The main area shows the "Rotations" panel content, including a text box with the instruction: "You can rotate the model around, but don't forget about the Undo half." Below this, there are sections for "Panel commands" and "Undo commands", both containing the command "turn y 2 90 ; wait".
- UCSF Chimera**: This panel shows the "Rotations" panel content, including the same text box and a small icon of the UCSF Chimera logo.

illustrations



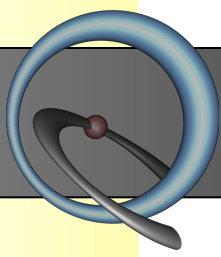
Questions?





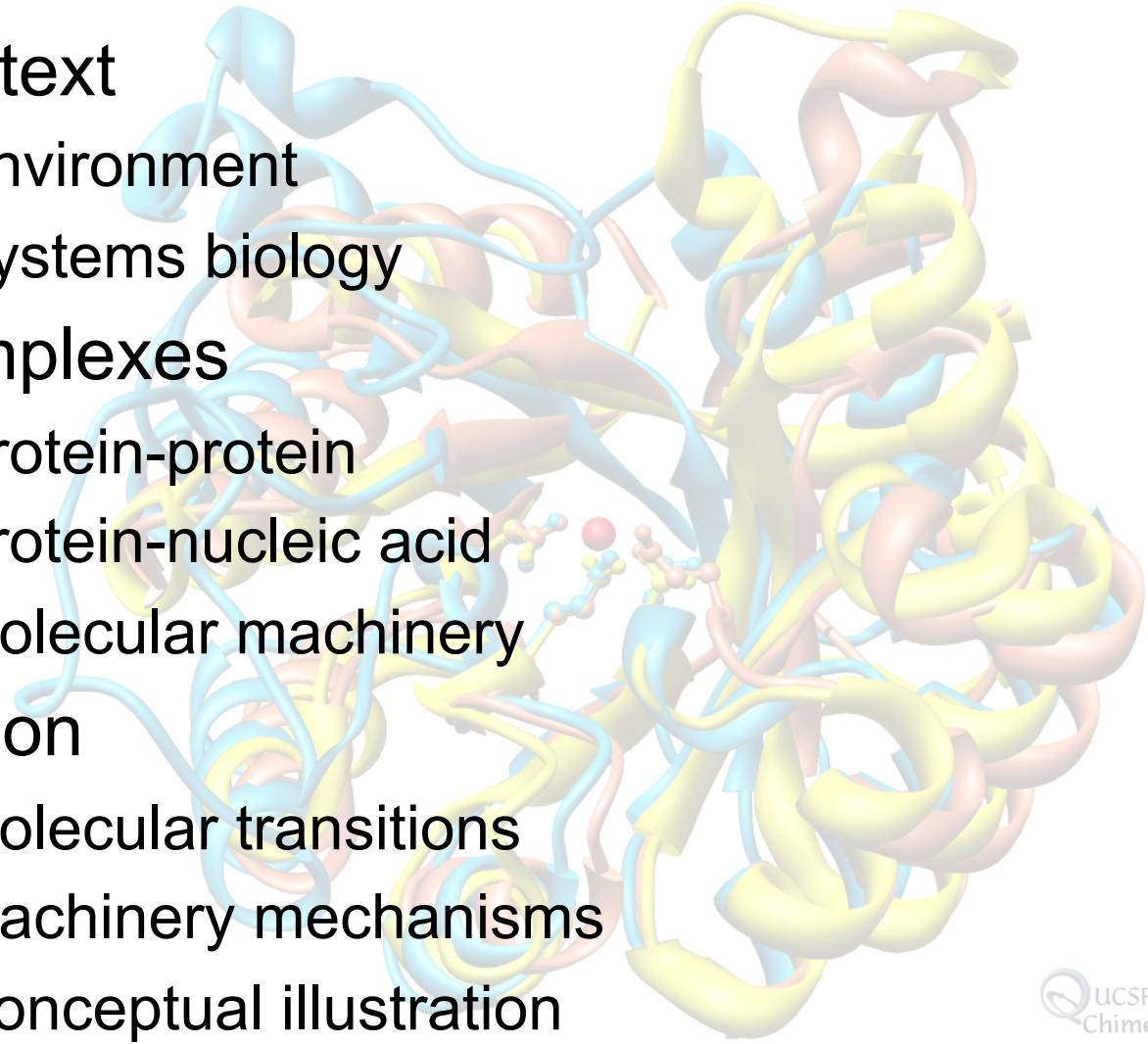
Chimera Recent Additions

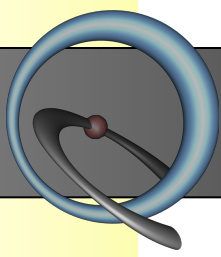
- **Modeling**
 - Rotamers
 - Fetch modeled structures from ModBase
 - Web service interface to Modeller and IMP
 - Web service interface to BLAST
- **Animation and illustration**
 - Movies can now be rendered with POVray
 - Scenes and Storyboards
- **Volume visualization**
 - New tools for tomographic data
- **Systems biology**
 - *structureViz*: links Cytoscape to Chimera



Visualization Directions

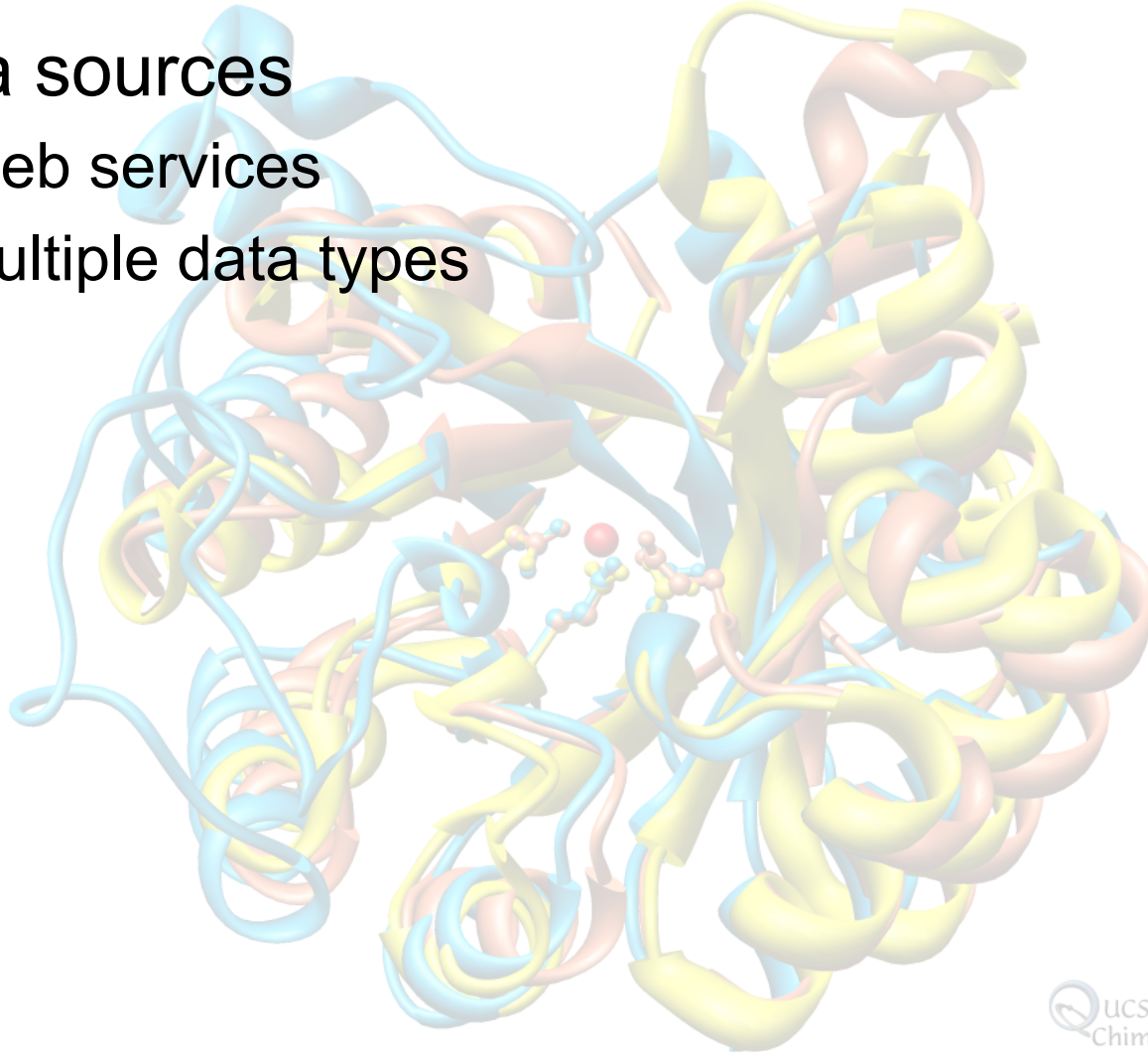
- Context
 - Environment
 - Systems biology
- Complexes
 - Protein-protein
 - Protein-nucleic acid
 - Molecular machinery
- Motion
 - Molecular transitions
 - Machinery mechanisms
 - Conceptual illustration

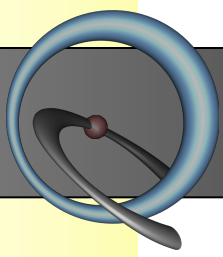




Visualization Directions

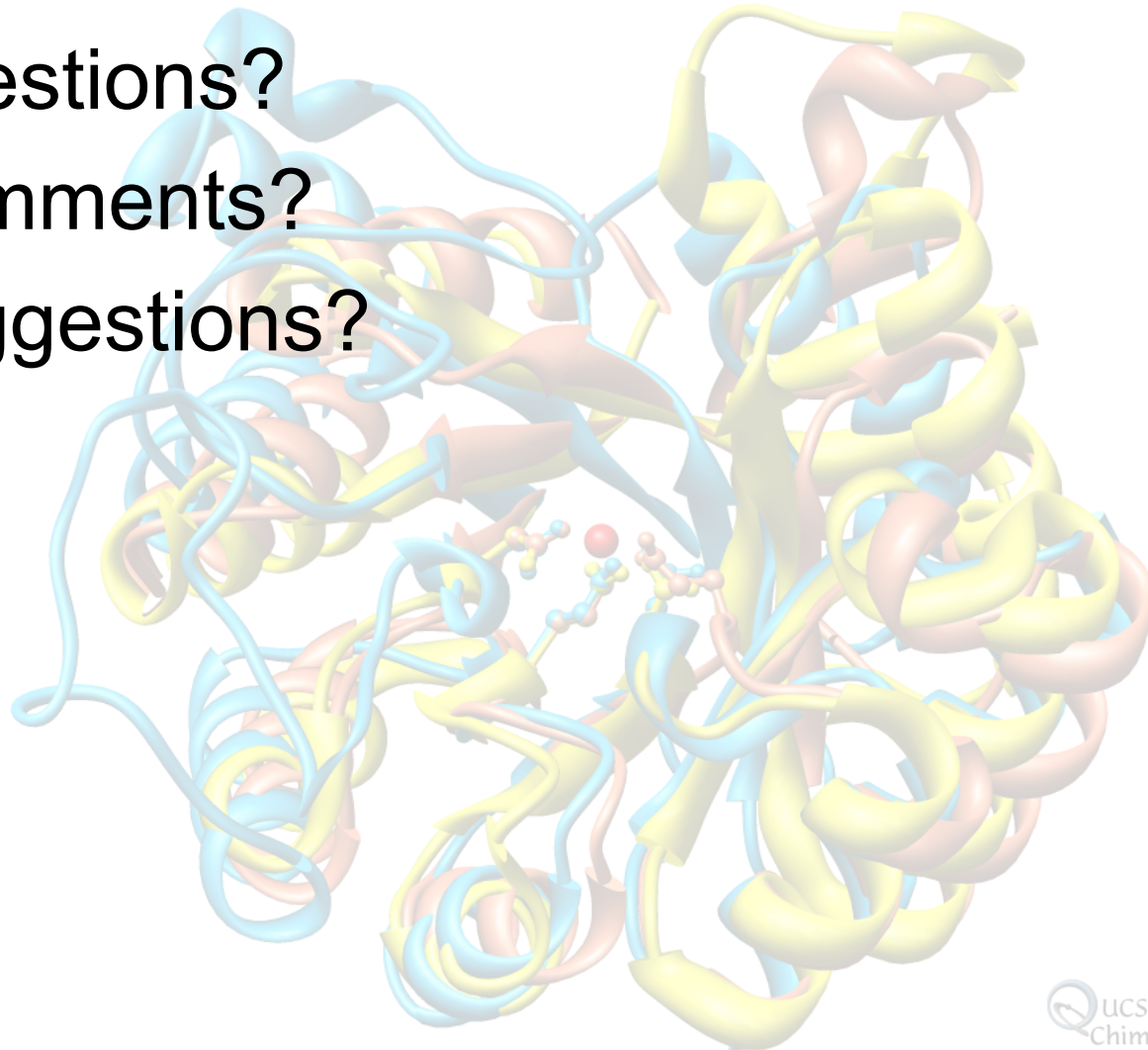
- Data sources
 - Web services
 - Multiple data types

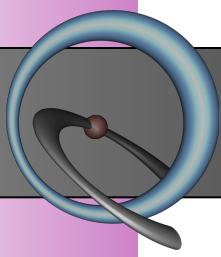




The End

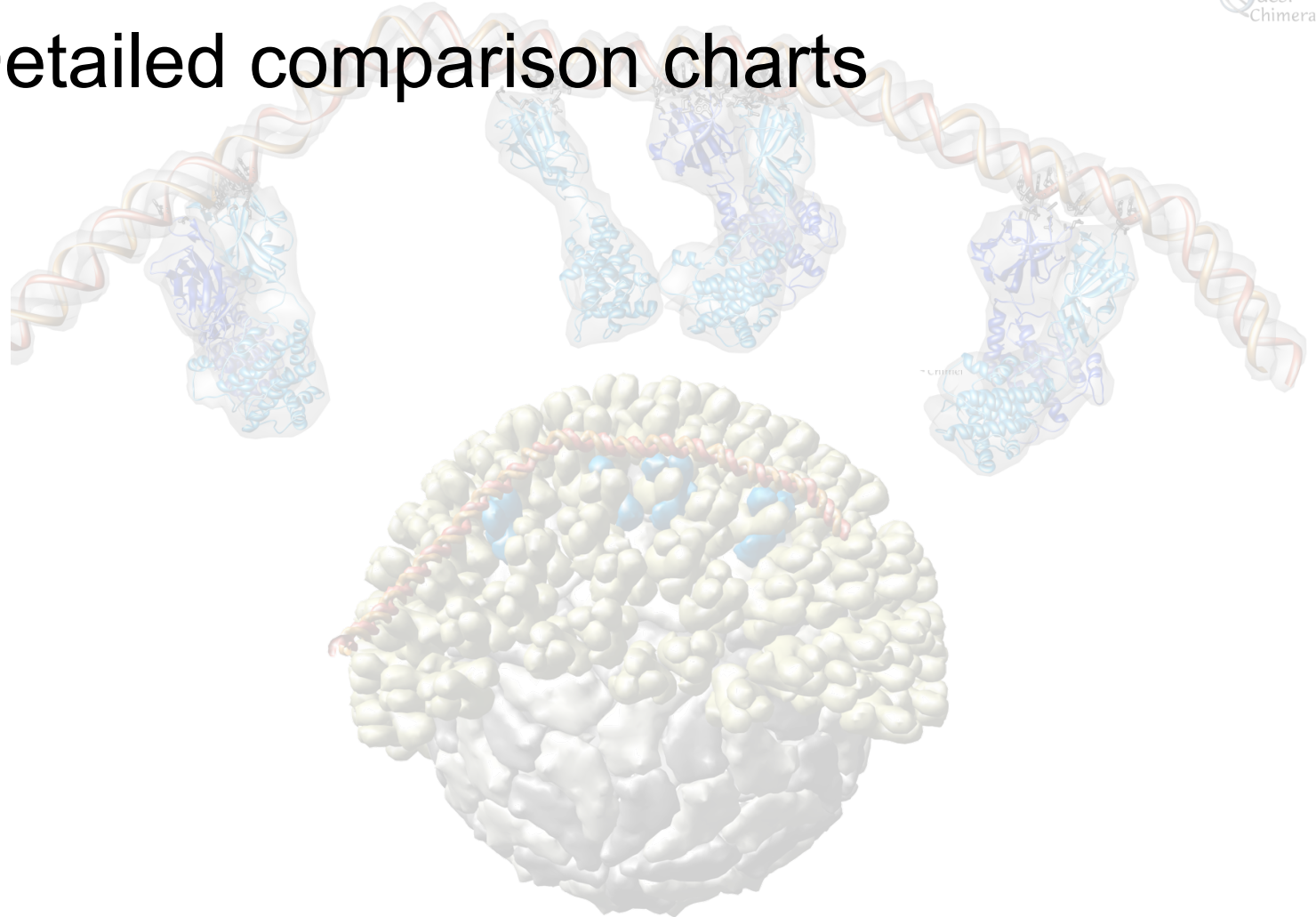
- Questions?
- Comments?
- Suggestions?





Backup Slides

- Detailed comparison charts



feature	Chimera 1.2199	RasMol 2.7.3	Jmol 10.2	PyMol 0.99	Deep View 3.7	VMD 1.8.4	DINO 0.9.1	Molmol 2K. 2
PDB	I/O	I/O		I/O	I/O	I/O	I/O	I/O
Mol2	I/O		-		-	I/O	-	
CIF/mmCIF	-			-	-	-	-	-
Web app	-	PE	+	-	-	-	-	-
sessions	+	-	-	+	+	+	-	+
color editing	+	-	-	+	+	+	-	+
transparency	+	-	+	+	SG	SD	+	-
molecular surfaces	+	+	+	+	+	+	DR	+
interface surfaces	+	-	-	-	-	+	-	-
solid clipped surface	+	+	-	-	-	PV	+	-
arbitrary clipping	+	-	-	-	-	+	+	-
movable labels	2D	-	-	+	-	-	-	+
special nucleic disp	+	-	-	+	-	+	+	+
geometric objects	+	-	+	+	-	+	-	+
high-quality images	+	-	-	+	-	-	+	+
ray-tracing support	+	+	+	++	+	+	+	+
stereo	+	+	+	+	+	++	+	+
multiscale/low-res	+	-	-	-	-	LR	-	SH
volume isosurfaces	++	-	+	+	+	+	+	+
transparent volumes	+	-	-	-	-	-	-	-
edit/write vol data	+	-	-	-	-	-	-	-
auto fit to density	+	-	-	-	-	-	-	-
measure volume	+	-	-	-	-	-	-	-

feature	Chimera 1.2199	RasMol 2.7.3	Jmol 10.2	PyMol 0.99	Deep View 3.7	VMD 1.8.4	DINO 0.9.1	Molmol 2K. 2
atom type ident	+	-	-	-	-	-	-	-
select AA category	+	+	FG/ST	-	+	+	+	-
H addition	+	-	-	SA	SA	SM	-	SR
H-bond ident	++	+	FG	+	+	+	-	+
charge assignment	SR	-	-	SR	SA	SM	-	SR
ESP calculation	ID/DR	CL	-	AP/DR	CL/PB	AP/DR	DR	PB
AA rotamer library	-	-	-	+	+	-	-	-
energy minimization	-	-	-	-	+	NM	-	-
render by attribute (e.g. color bfactor)	++	+	+	+	+	+	+	+
user-defined attribs	+	-	-	-	-	-	-	-
seq align viewer	++	SP	SP/ST(I)	SP	IG	SP/IG	-	-
seq-based match	+	-	-	+	+	-	-	-
struct-based match	+	-	-	SP	+	+	-	-
seq align from match	+	-	-	-	PW	+	-	-
MD playback	+	-	PO	+	-	++	+	PO
view docking results	+	-	-	-	-	-	-	-
context/balloon help	+	-	+	-	-	-	-	+
user docs	++	+	+	OD	+	+	+	++
programming docs	+	-	-	-	+	+	-	-
extensibility	+	-	+	+	-	+	-	-
source distrib	+	+	+	+	-	+	-	+
platforms	W/M/U	W/M/U	W/M/U	W/M/U	W/M/U	W/M/U	M/U	W/U

I input

O output

- feature not present

+ feature present

++ feature present and comparatively extensive or sophisticated

PE Protein Explorer { #52} is a Web application based on RasMol

SG only surfaces and only on Silicon Graphics

SD “screen door” transparency

DR displays results from other programs

PV non-interactive solid-color clip available via POV ray-tracer

2D arbitrary labels can be created and moved in the plane of the screen

SH only certain shapes (rectilinear boxes, spheres, ellipsoids)

FG via FirstGlance in Jmol (<http://firstglance.jmol.org>)

ST via STING { #56} (<http://www.cbi.cnptia.embrapa.br/SMS/>); (I) = Windows/Intel Linux only and only alignments from STING-related databases

SA residues with topology files in the distribution (standard amino acids and a few others)

SM small structures only

SR residues in the AMBER 94 library { #77} (used in the ff94-ff99 versions of the force field)

ID interface to DelPhi { #75; #76} (obtained separately)

CL Coulomb’s law calculation

PB Poisson-Boltzmann calculation

AP interface to Adaptive Poisson-Boltzmann Solver { #74} (obtained separately)

NM via input to/output from NAMD { #73}

SP STRAP plug-in { #49}, <http://www.charite.de/bioinf/strap/> (Java); according to the author, interfacing to RasMol and VMD may only work on Unix, and only PyMol shows structure superpositions from STRAP (see <http://www.charite.de/bioinf/strap/pymol.html>)

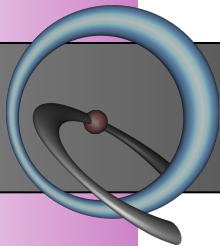
IG internally generated alignments

PW pairwise comparisons only; adjusts one sequence relative to one other

PO PDB-format input only

OD out-of-date user manual supplemented with mailing list and volunteer-provided tutorials and wiki

platforms: W Windows, M Macintosh, U Unix



Backup



RasMol { #53; #54} : <http://www.bernstein-plus-sons.com/software/rasmol/>

Jmol { #32}: <http://jmol.sourceforge.net/>

PyMol { #29}: <http://pymol.sourceforge.net/>

Deep View (Swiss-Pdb Viewer) { #51}:<http://ca.expasy.org/spdbv/>

VMD { #24}: <http://www.ks.uiuc.edu/Research/vmd/>

DINO { #55}: <http://www.dino3d.org/>

Molmol { #48}: <http://hugin.ethz.ch/wuthrich/software/molmol/>