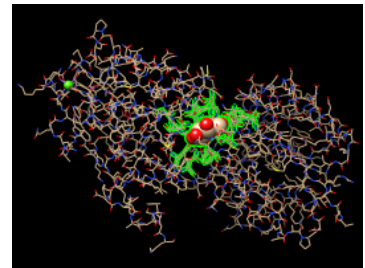


Analyzing and Comparing Structures with UCSF Chimera

- Demonstration (~20 mins):
 - general concepts and tips for using Chimera
 - preview of some of the tools you will be using
 - OK (preferable?) to watch rather than trying to follow along; if you do try things, close session or quit/restart before starting the tutorial
 - Hands-on tutorial:
 - **Structure Analysis and Comparison** (~45 minutes)
 - Optional tutorials (available from **Help** menu):
 - **Attributes** (~20 minutes)
 - **Trajectory and Ensemble Analysis** (~35 minutes)
 - **The Model Panel and Ensembles** (~20 minutes)
-

Turning Data into Information

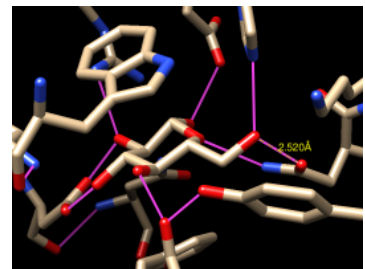
- molecular graphics as an analysis tool
- visual presentation of information carried in atomic coordinates
- mapping non-coordinate information onto graphics



Demonstration Outline

General concepts, basic structure analysis:

- customizing tool startup and icons with **Preferences**
- zone selection
- measuring a distance
- identifying hydrogen bonds (**FindHBond**)
- commands and atom specification symbols
- command help, **Help** buttons, **Help** menu
- documentation is local (included in download) and searchable



Structure comparison:

- superimposing structures with **MatchMaker**
- morphing between different conformations
- viewing and recording a morph trajectory with **MD Movie**



Attributes (atom and residue property values):

- showing B-factor with colors using **Render by Attribute**
- showing amino acid hydrophobicity with "worms"
- attributes can be used in commands
- users can define custom attributes in a simple text format
- various operations in Chimera also create attributes (surface area, conservation in an alignment, etc.)

