Visualization of biomolecules with VMD

Visualization Programs:

Name	Organization	Link
VMD	U Illinois	http://www.ks.uiuc.edu/Research/vmd/
jmol	OpenScience	http://jmol.sourceforge.net/
Pymol	Schroedinger Inc	http://www.pymol.org/
MOE	CCG Inc.	http://www.chemcomp.com/
DS	Accelrys Inc.	http://www.accelrys.com/

Visual Molecular Dynamics (VMD)

Web page:
http://www.ks.uiuc.edu/Research/vmd/

Developers

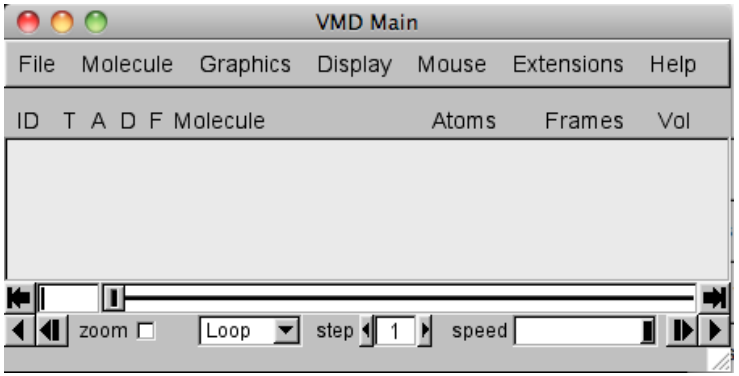
Schulten group, University of Illinois at Urbana Champaign, USA

Functionalities: Molecular Modeling

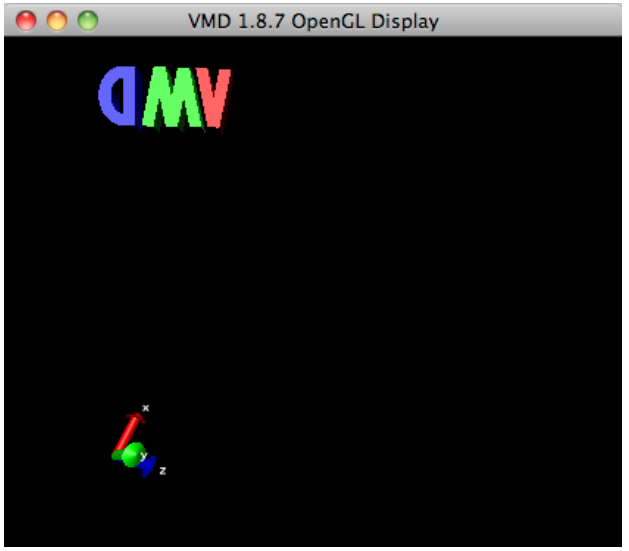
- Complex graphical representation of molecules (focus on proteins)
- Animation of trajectories
- Generation of NAMD input files

Start of VMD

- Start by typing "*vmd*" in the terminal window
- Successful start brings up **three windows**

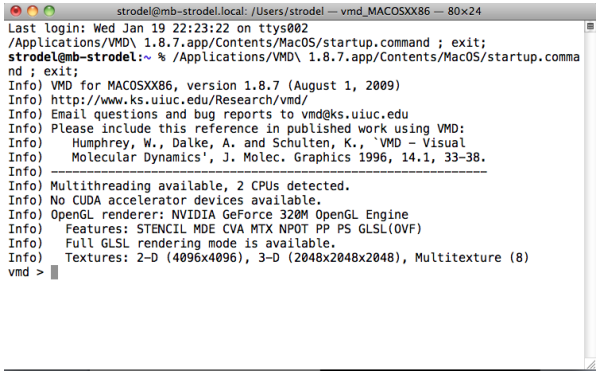


Main window



Graphics window

Console window



Tasks:

- How to use the terminal in Linux (Linux basic commands)
- Learning the usage of the visualization program VMD
- Becoming familiar with Protein Data Bank
- Answer all questions in the following sites

Task: Visualizing a protein

Object of study: β-lactamase proteins

- Investigate active site of a β-lactamase II from *Bacillus cereus*:

  PDB code **3BC2**

- Using a web browser, go to **PDB database**: http://www.rcsb.org
- The **Protein Data Bank (PDB)** is a database for the three-dimensional structural data of large biological molecules, such as proteins and nucleic acids.
- Enter **3BC2** into search field, invoke "*Search*":

Q1: *What secondary structure elements can one already see on the web page?*

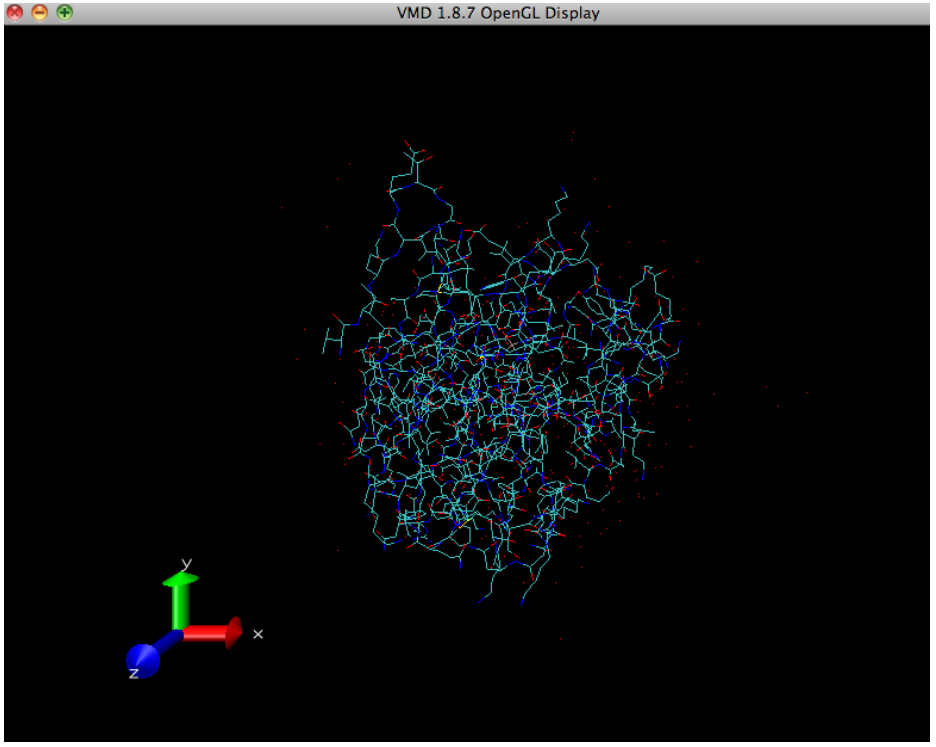
Q2: *What is the expected sequence length?*

Q3: *What ligands are reported?*

- Download the PDB file (as Text) and save it somewhere.

Loading a structure in VMD

- Open **3BC2.pdb** via *Main Window* > *File* > *New Molecule*
- *Browse* to file **3BC2.pdb** and click *load*.
- The Graphics Window should look like:



- The basic view is showing the chemical bonds as *lines* (with *element coloring*)

Q4: *Inspecting some chemical groups, what is missing?*

Basic commands for viewing in VMD

The *Graphics Window* has ca. three basic **mouse operation modes**:

- **Rotation** mode (default):

  type *r* or go to *Main Window* > *Mouse* > *Rotate Mode*

- **Translation** mode:

  type *t* or go *Main Window* > *Mouse* > *Translate Mode*

- **Scale** mode:

  type *s* or go *Main Window* > *Mouse* > *Scale Mode*

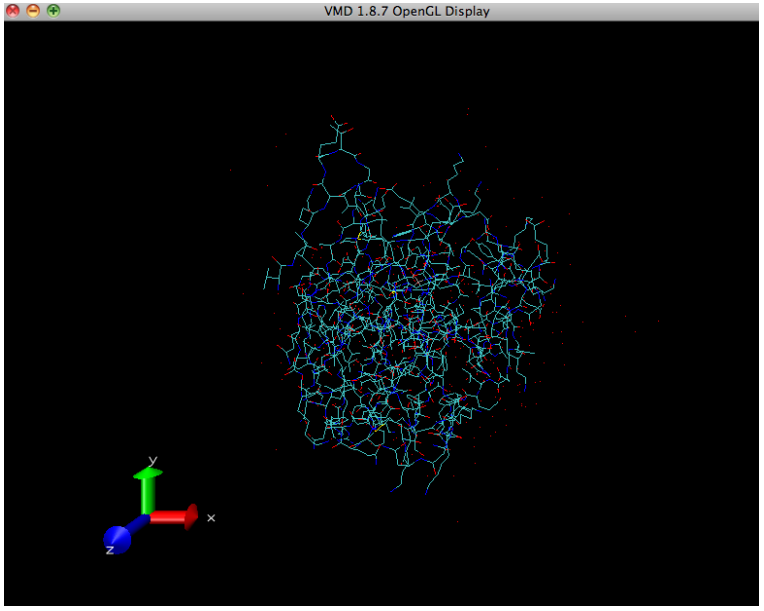
Notes:

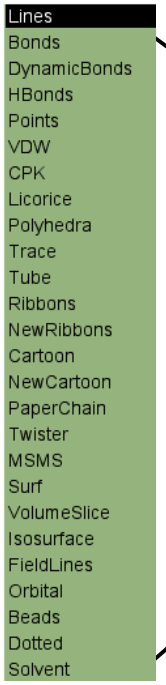
- These operations are “passive”, i.e. they do not change the coordinates of the system
- Reset the view by *Main Window* > *Display* > *Reset View*

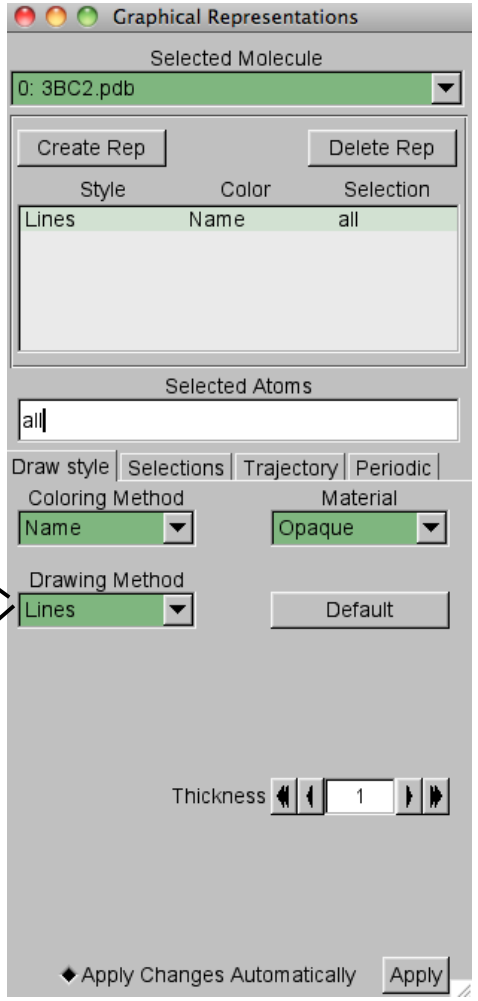
Visualization styles in VMD

- Go to *Main Window* > *Graphics* > *Representations*

These styles apply to the current representation (see next slide)



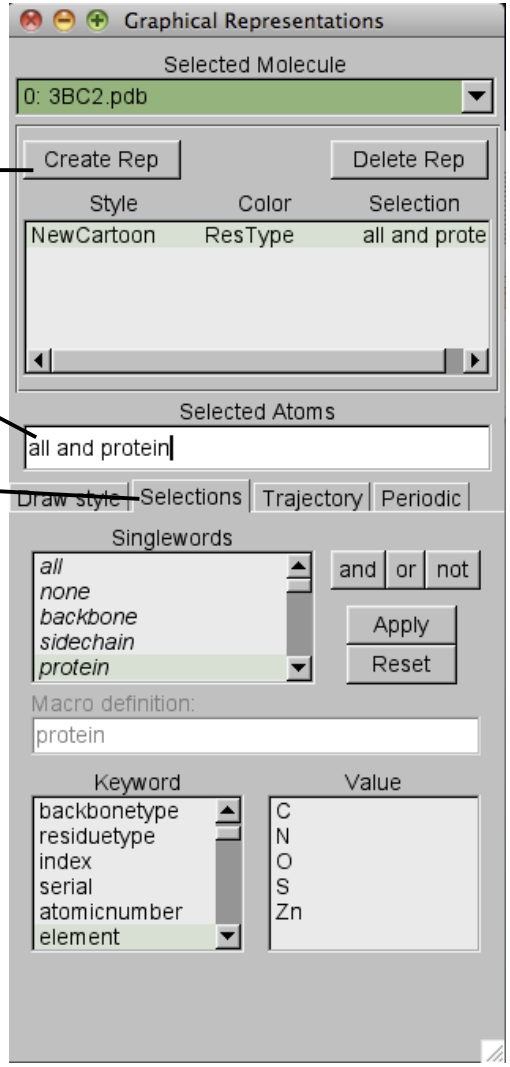




- Try various **Drawing Methods** and **Coloring Methods**.
- At the end: Turn to *New Cartoon* with coloring *ResType*

Atomic selections in VMD

- To change set of atoms to which *Draw Style* applies, a **selection** command is entered.
- Selections may be typed-in or composed by choosing from *Selections > Singlewords*, *Keywords* and *Values.*
- *Create Rep* creates a copy of the current drawing.
- Try and create various representations with different selections.



Task: Atomic selections

Q5: *Describe what and how is displayed applying the following selections and drawing methods (you may create new representations)*:*

selection	drawing method
protein	*New Cartoon*
element Zn	*New Cartoon (or Lines, or Bonds)*
element Zn	*vdW (or CPK)*
within 5.0 of element Zn	*CPK*
same residue as within 5.0 of element Zn	*CPK*

* Please describe exactly what you see in the 1-2 sentences (optionally with a picture).

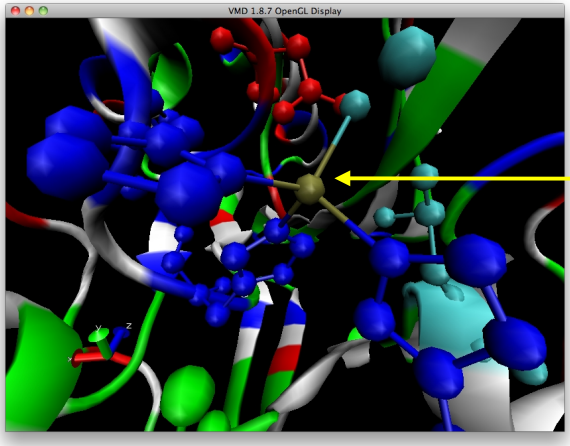
Picking & Labeling atoms

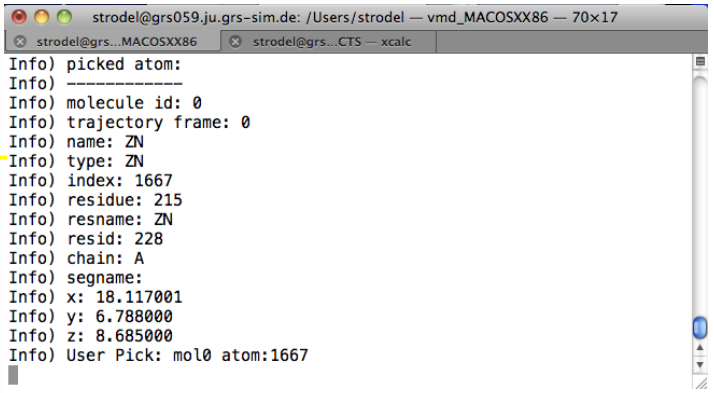
This helps to identify atoms:

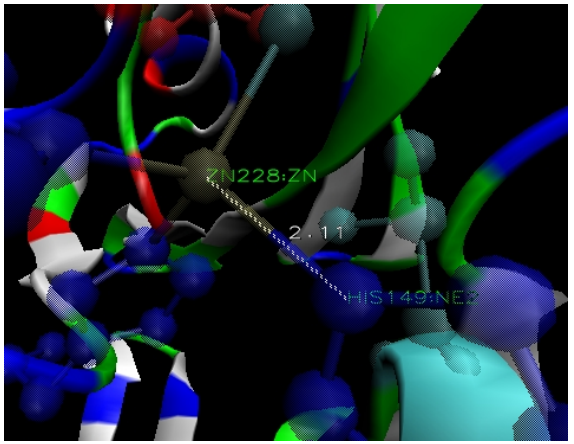
- **Picking:** *Main window > Mouse > Pick*
  shows information of atom clicked at in the Console Window.
- **Labeling:** *Main Window > Mouse > Label > {Atoms, Bonds, Angle Dihedral}*
  picks atoms and puts text into the graphics windows

Notes:

- Label colors may be set through *Main Window > Graphics > Colors > Categories > Labels*
- Labels may be hidden, deleted or re-shown through *Main Window > Graphics > Labels*







Exporting & Saving in VMD

- **Saving VMD state** (to continue at same point):

  Main Window > *File* > *Save State*

  Choose file name ending with *.vmd*

- **Exporting graphical display**:

  Main Window > *File* > *Render*

  Export as *.tga* using snapshot.

Further Tasks

Q6: *What molecules/residues is the zinc ion binding to (residue type and number)?*

Q7: *Label all binding distances of zinc (distance and to which residue).*

Q8: *Is the zinc binding geometry tetrahedral? Prove and explain it with the angle description.*

(Hint: Measure the angles between the zinc atoms and its binding atoms)

Q9: *Save a picture of the zinc binding site.*

(Hint: Change background color to *white* via *Main Window* > *Graphics* > *Colors* > *Categories* > *Display* > *Names* > *Background.*)

- **Save all your answers to the questions** in an *Openoffice/word* text document and **include the figure from Q9** (call it via *ooffice* using terminal shell) .
- **Send the document to** *b.strodel@fz-juelich.de*.
- Include your **name in the document**!