

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

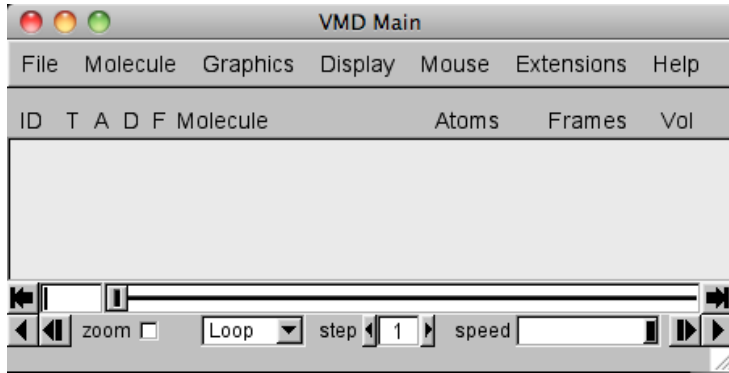
Schulten group, University of Illinois at Urbana Champaign, USA

Functionalities: Molecular Modeling

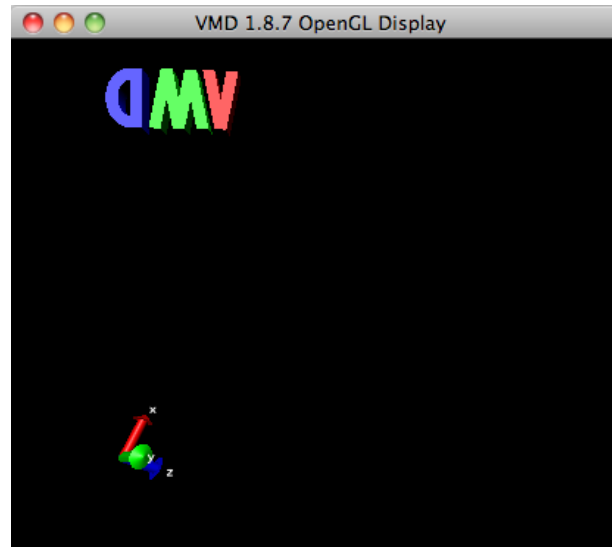
- Complex graphical representation of molecules (focus on proteins)
- Animation of trajectories
- Generation of NAMD input files

Start of VMD

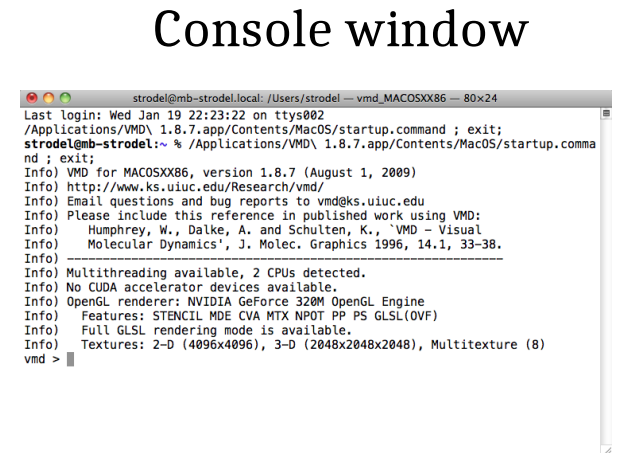
- Start by typing “vmd” in the terminal window
- Successful start brings up **three windows**



Main window



Graphics window



- 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*”:



The image shows a search bar from the Protein Data Bank (PDB) website. The search bar is a light blue rectangle with a white input field. Inside the input field, the text '3BC2' is entered. To the left of the input field, there is a dropdown menu with the text 'PDB ID or Text' and a small blue arrow pointing down. To the right of the input field, there is a rounded rectangular button with the text 'Search' in a light blue font. The background of the search bar is a solid blue color.

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

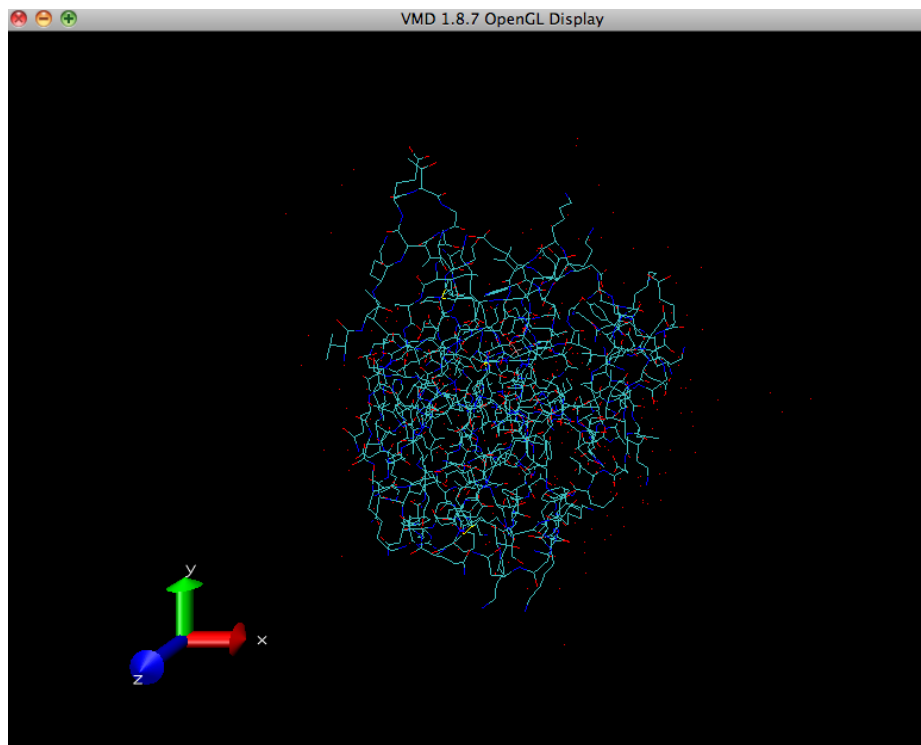
Q2: *What is the expected sequence length?*

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*

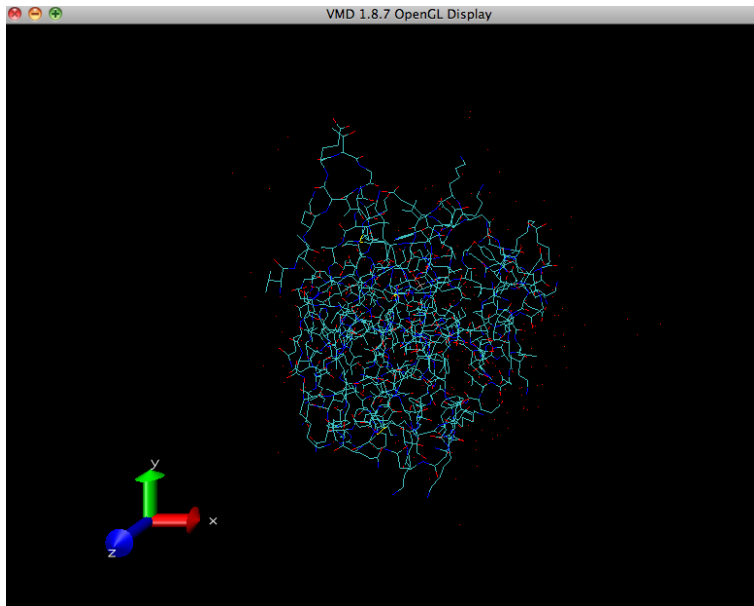
Notes:

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

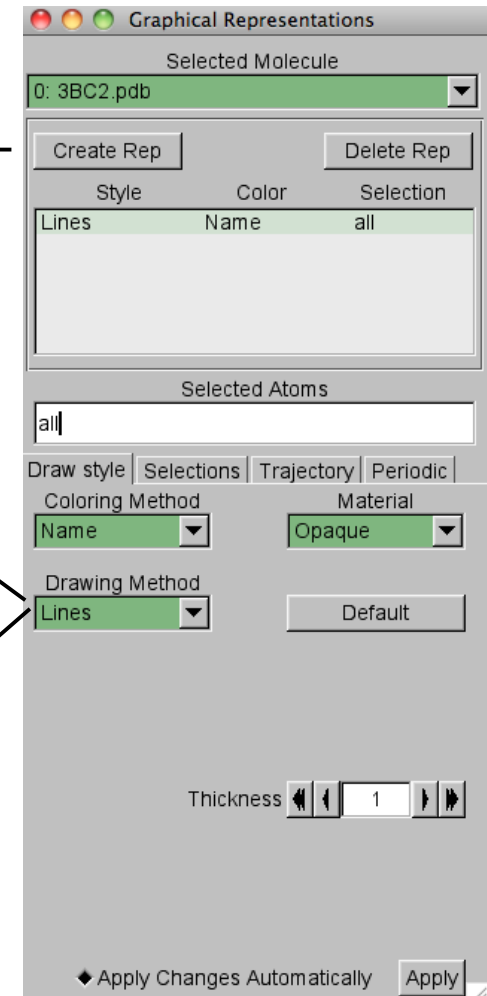
Visualization styles in VMD

- Go to *Main Window > Graphics > Representations*

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



- Lines
- Bonds
- DynamicBonds
- HBonds
- Points
- VDW
- CPK
- Licorice
- Polyhedra
- Trace
- Tube
- Ribbons
- NewRibbons
- Cartoon
- NewCartoon
- PaperChain
- Twister
- MSMS
- Surf
- VolumeSlice
- Isosurface
- FieldLines
- Orbital
- Beads
- Dotted
- Solvent



Graphical Representations

Selected Molecule
0: 3BC2.pdb

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all

Selected Atoms
all

Draw style Selections Trajectory Periodic

Coloring Method Material
Name Opaque

Drawing Method
Lines Default

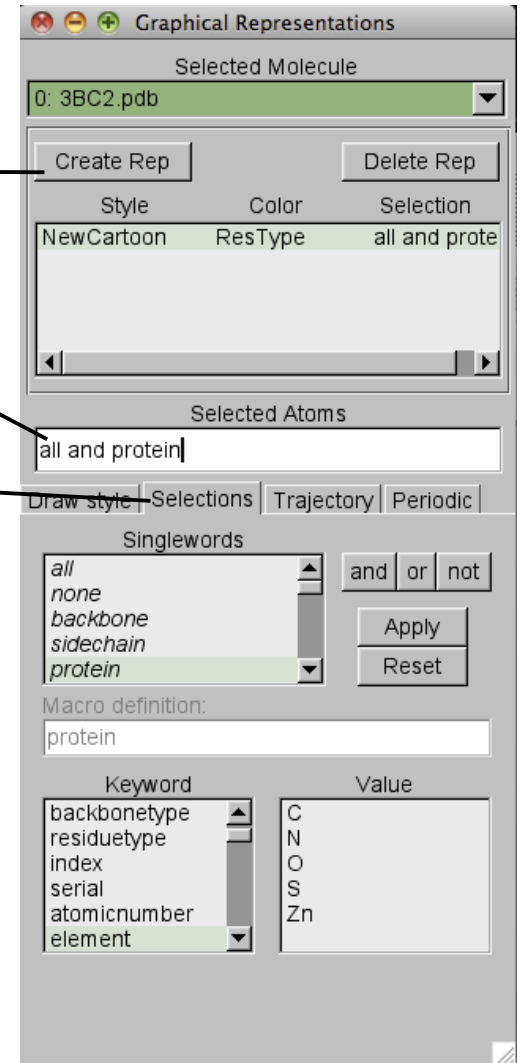
Thickness 1

Apply Changes Automatically Apply

- 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)*:

<u>selection</u>	<u>drawing method</u>
<i>protein</i>	<i>New Cartoon</i>
<i>element Zn</i>	<i>New Cartoon (or Lines, or Bonds)</i>
<i>element Zn</i>	<i>vdW (or CPK)</i>
<i>within 5.0 of element Zn</i>	<i>CPK</i>
<i>same residue as within 5.0 of element Zn</i>	<i>CPK</i>

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

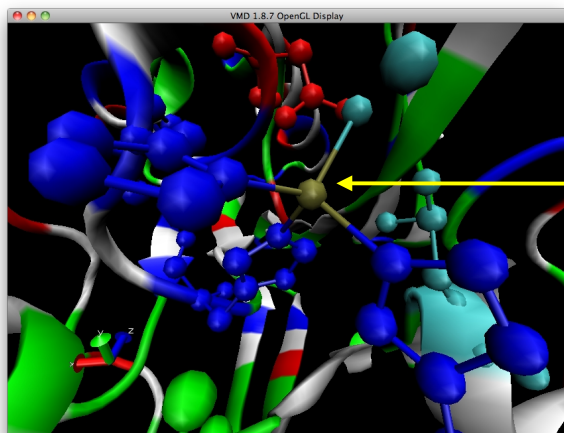
Picking & Labeling atoms

This helps to identify atoms:

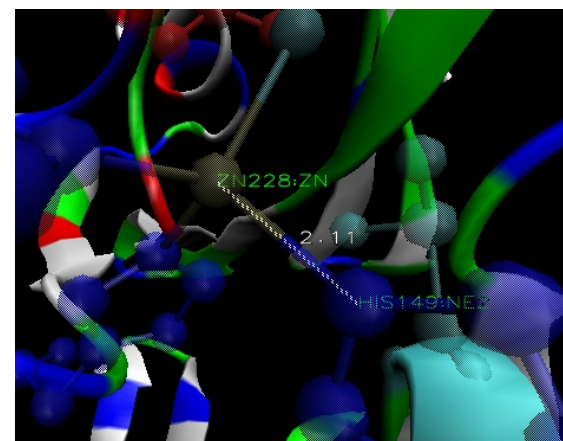
- **Picking:** *Main window > Mouse > Pick* shows information of atom clicked at in the Console Window.
- **Labeling:** *Main Window > Mouse > Label > {Atoms, Bonds, Angle Dihedral}* picks atoms and puts text into the graphics windows

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*



```
strodel@grs059.ju.grs-sim.de: /Users/strodel — vmd_MACOSX86 — 70x17
strodel@grs...MACOSX86  strodel@grs...CTS — xcalc
Info) picked atom:
Info) -----
Info) molecule id: 0
Info) trajectory frame: 0
Info) name: ZN
Info) type: ZN
Info) index: 1667
Info) residue: 215
Info) resname: ZN
Info) resid: 228
Info) chain: A
Info) segname:
Info) x: 18.117001
Info) y: 6.788000
Info) z: 8.685000
Info) User Pick: mol0 atom:1667
```



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!**