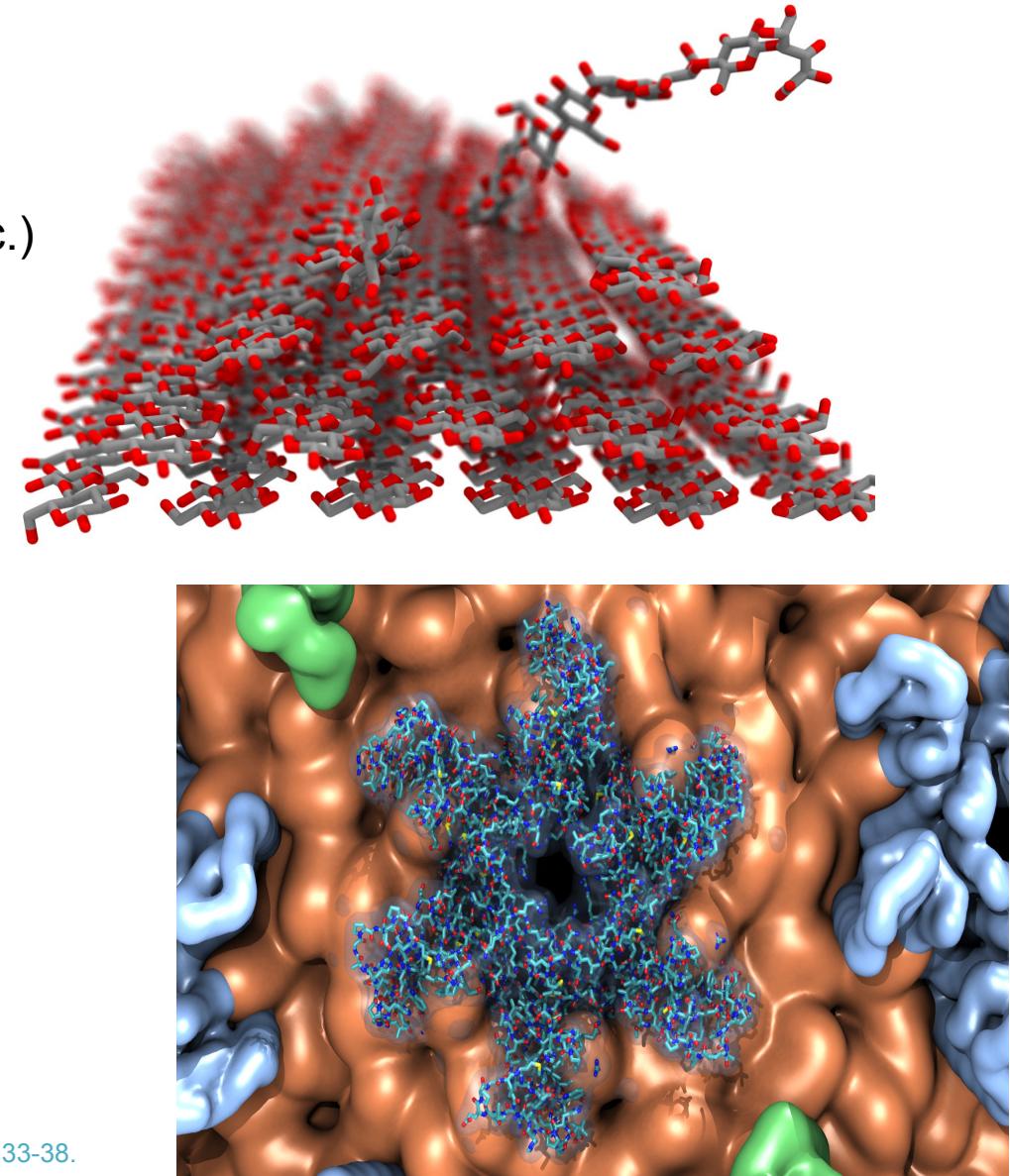
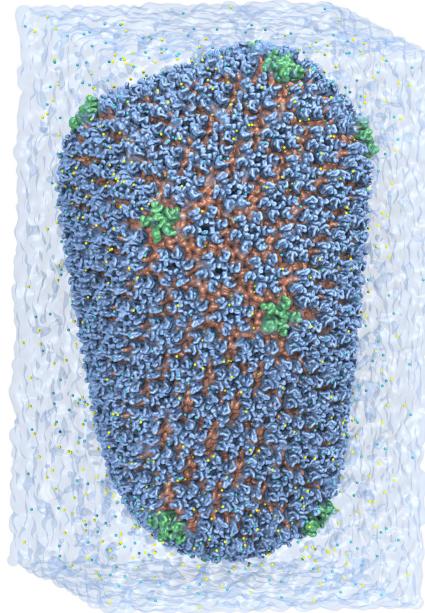


# Introduction to VMD (Visual Molecular Dynamics)

- Visualizing large Molecular Dynamics Trajectories
- Supports many molecular formats (PDB, PSF, DCD, etc.)
- Commonly used with NAMD and CHARMM
- Open-source and cross-platform
- Data Analysis tools
- HD images and Movie making
- Built in tcl and python scripting



# Installing VMD on Linux OS

## 1. Go to Download: [www.ks.uiuc.edu/Research/vmd](http://www.ks.uiuc.edu/Research/vmd)

### Version 2.0.0 LATEST ALPHA (2025-03-13) Platforms:

Latest pre-release ALPHA test version

- LINUX\_64 (RHEL 8+) OpenGL, CUDA, OptiX RTX, RTX RTF

### Version 1.9.4 LATEST ALPHA (2023-06-08) Platforms:

Latest pre-release ALPHA test version

- Source Code
- LINUX\_64 (RHEL 7+) OpenGL, CUDA, OptiX RTX, OSPRay
- LINUX\_64 (RHEL 7+) OpenGL, CUDA, OptiX RTX, OSPRay,
- MacOS 11.x, ARM64 (64-bit "M1" Macs) (Apple MacOS-X 11)
- MacOS 10.15, x86\_64 (64-bit Intel x86\_64) (Apple MacOS-X)
- Windows 64-bit, CUDA, OptiX, OSPRay (64-bit Intel x86\_64)



## 2. Register

### Registration/Login

You will need a username and password to download software.

If this is your first download, please choose a username and password to register.  
Current NAMD or VMD users, please enter your existing username and password.

Username:

Password:

Your download will continue after you have registered or logged in.

## 3. VMD folder contents

```
di97gef@badwlrz-cl18014:~/vmd-1.9.4a57$ ls
Announcement      distrib    msvc      scripts
bin                doc        plugins   shaders
configure          lib        proteins  src
configure.options  LICENSE   python
data               LINUXAMD64 README
```

## 4. modify configure file (optional)

```
#####
# User modifiable installation parameters, can be overridden by env variables
#####
# Name of shell script used to start program; this is the name used by users
$install_name = "vmd";

# Directory where VMD startup script is installed, should be in users' paths.
$install_bin_dir="/home/di97gef/.local/bin/";

# Directory where VMD files and executables are installed
$install_library_dir="/home/di97gef/Documents/packages/vmd/";
```

# Installing VMD on Linux OS

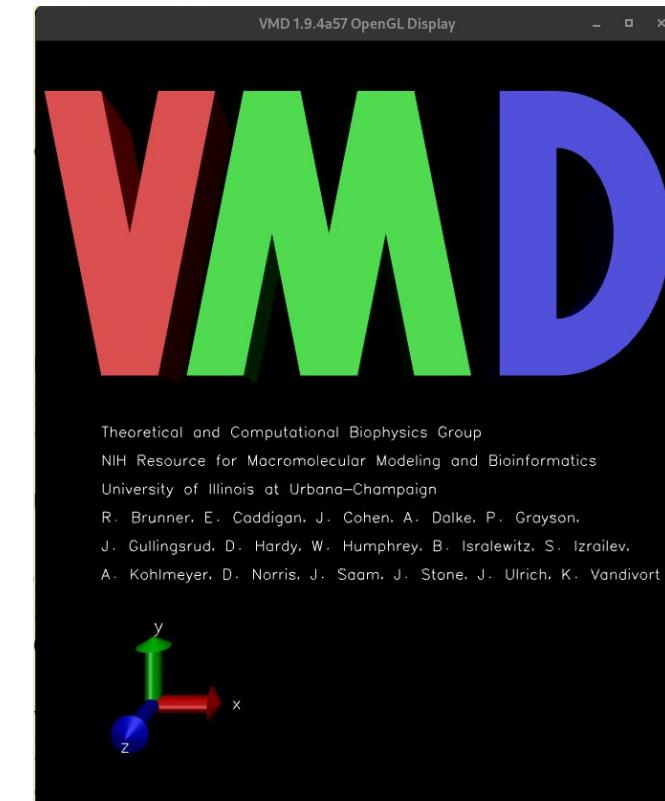
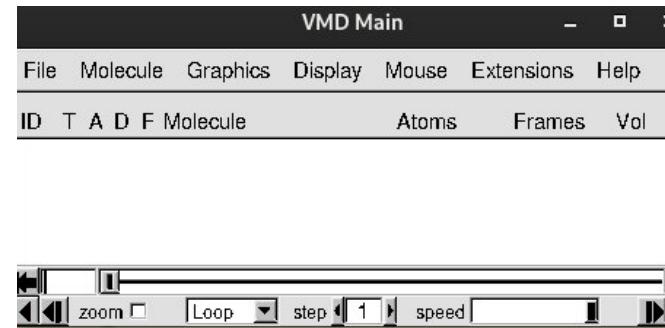
```
# Architectures:
# -----
# AIX6_64      - compile on an RS/6000 machine (gcc/g++/xlc/xlc)
# ANDROIDARMV7A - cross-compile for Android on ARM V7A
# BLUEWATERS   - compile for NSF/NCSA Blue Waters
# CRAY_XC      - compile for Cray XCx0 machines with GPUs
# CRAY_XK      - compile for Cray XKx machines with GPUs
# FREEBSD       - compile on a FreeBSD machine (gcc/g++)
# FREEBSDAMD64 - compile on a FreeBSD machine (gcc/g++)
# LINUX        - compile on a Linux machine (x86 32-bit)
# LINUXAMD64   - compile on a Linux machine (x86 64-bit AMD64 or EM64T)
# LINUXARM64   - compile on a Linux machine (64-bit ARM)
# LINUXPPC64   - compile on a Linux machine (64-bit PowerPC)
# MACOSX       - compile on a MacOS-X PowerPC machine
# MACOSXARM64  - compile on a MacOS-X ARM64 machine, 64-bit ABI
# MACOSXX86    - compile on a MacOS-X x86 machine, 32-bit ABI
# MACOSXX86_64 - compile on a MacOS-X x86 machine, 64-bit ABI
```

## 5. Run configure

```
di97gef@badwlrz-cl18014:~/vmd-1.9.4a57$ ./configure LINUXAMD64
```

## 6. Go to src folder and vmd install

```
di97gef@badwlrz-cl18014:~/src$ make install
if [ ! -d "/home/di97gef/Documents/packages/vmd/" ]; then \
    mkdir -p "/home/di97gef/Documents/packages/vmd/" ; \
fi ; \
if [ ! -d "/home/di97gef/.local/bin/" ]; then \
    mkdir -p "/home/di97gef/.local/bin/" ; \
fi ; \
if [ ! -d "/home/di97gef/Documents/packages/vmd//doc" ]; then \
    mkdir -p "/home/di97gef/Documents/packages/vmd//doc"; \
fi
```



# VMD in this course

<https://vm-138-246-237-46.cloud.mwn.de:8443/>

Leibniz Supercomputing Centre  
of the Bavarian Academy of Sciences and Humanities

integrated, single access point for all of your HPC

Desktop Apps

 noVNC

Remote Desktop Container

Development

 Code Server for VS Code

 Jupyter Notebook

Files

 Home Directory

System Installed App

remote Desktop Container

### Remote Desktop Container

This application uses noVNC to connect to a remote desktop session hosted within a container on a compute node, provided by a VNC server.

If a connection session has timed out, the button "Launch Remote Desktop" can be used to re-enter the session. Because of security concerns, attempting to rejoin directly from noVNC will not work.

Select a container image:

Rocky 9.3 | XFCE4 | Charliecloud | SquashFS

Select a cluster partition for your job: node-small

cpu@red-lion::node

Number of CPU nodes

1

Number of cores per job task on a single node - CPU flavor

Medium 8 cores

The real memory required per node - RAM flavor

Small 32 GB

Total run time in hours

1

Launch

\* The Remote Desktop Container session data for this session can be accessed under the [data root directory](#).



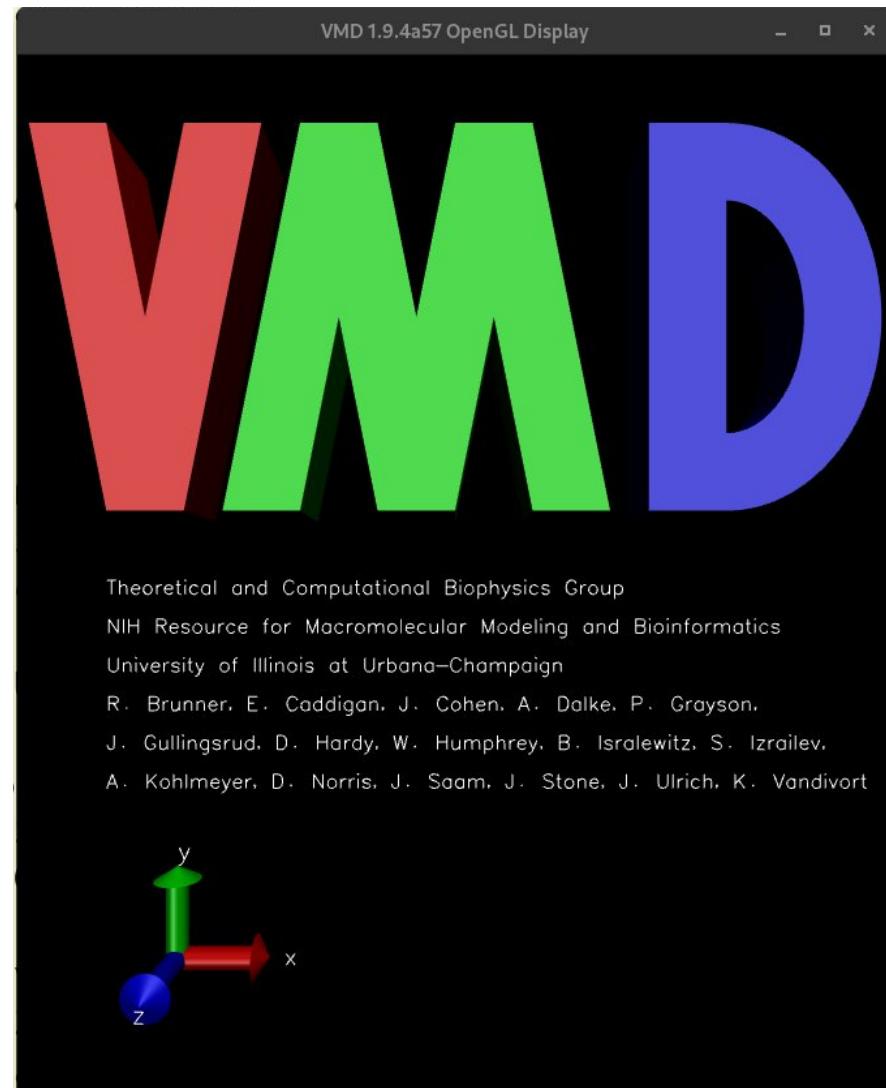
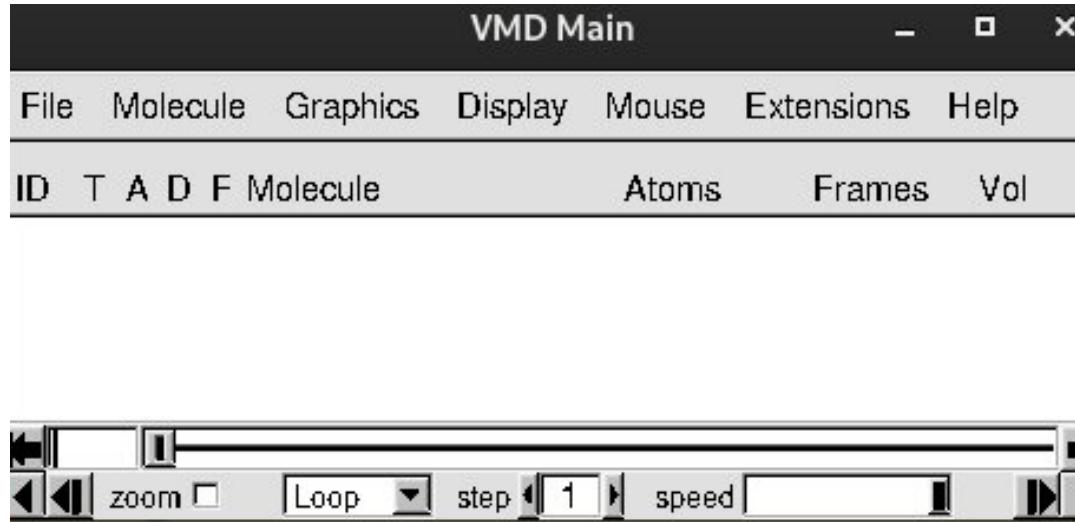
In addition to EESSI, other software is available at /custom\_software\_rocky/spack/shared/ux-rocky9-icelake

Course data is available at /course\_data

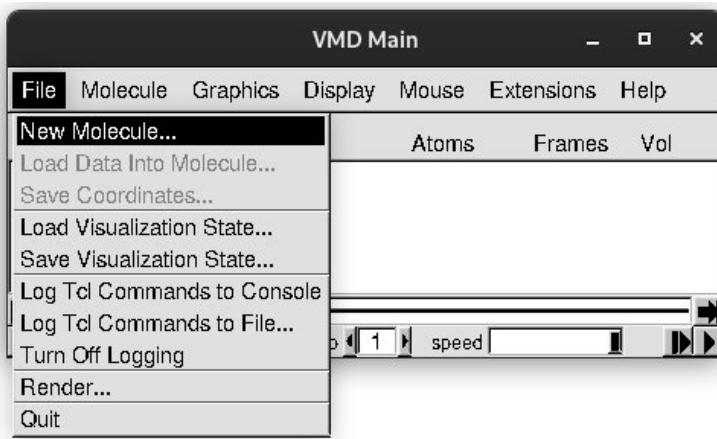
Backup your data to folder /backups/Up only required data.

```
[di97gef@node1 ~]$ module load vmd
[di97gef@node1 ~]$ vmd
```

# VMD in this course



# Supported Formats



**VMD Main**

**File** Molecule Graphics Display Mouse Extensions Help

- New Molecule...
- Load Data Into Molecule...
- Save Coordinates...
- Load Visualization State...
- Save Visualization State...
- Log Tcl Commands to Console
- Log Tcl Commands to File...
- Turn Off Logging
- Render...
- Quit

Atoms Frames Vol

speed [1] [◀ ▶]


**Molecule File Browser**

Load files for: New Molecule

Filename: **om\_software/course\_data/vmd/1ZEW.pdb**

Determine file type: **PDB**

Frames:

First: **0** Last: **-1** Stride: **1**

Load in background  
 Load all at once

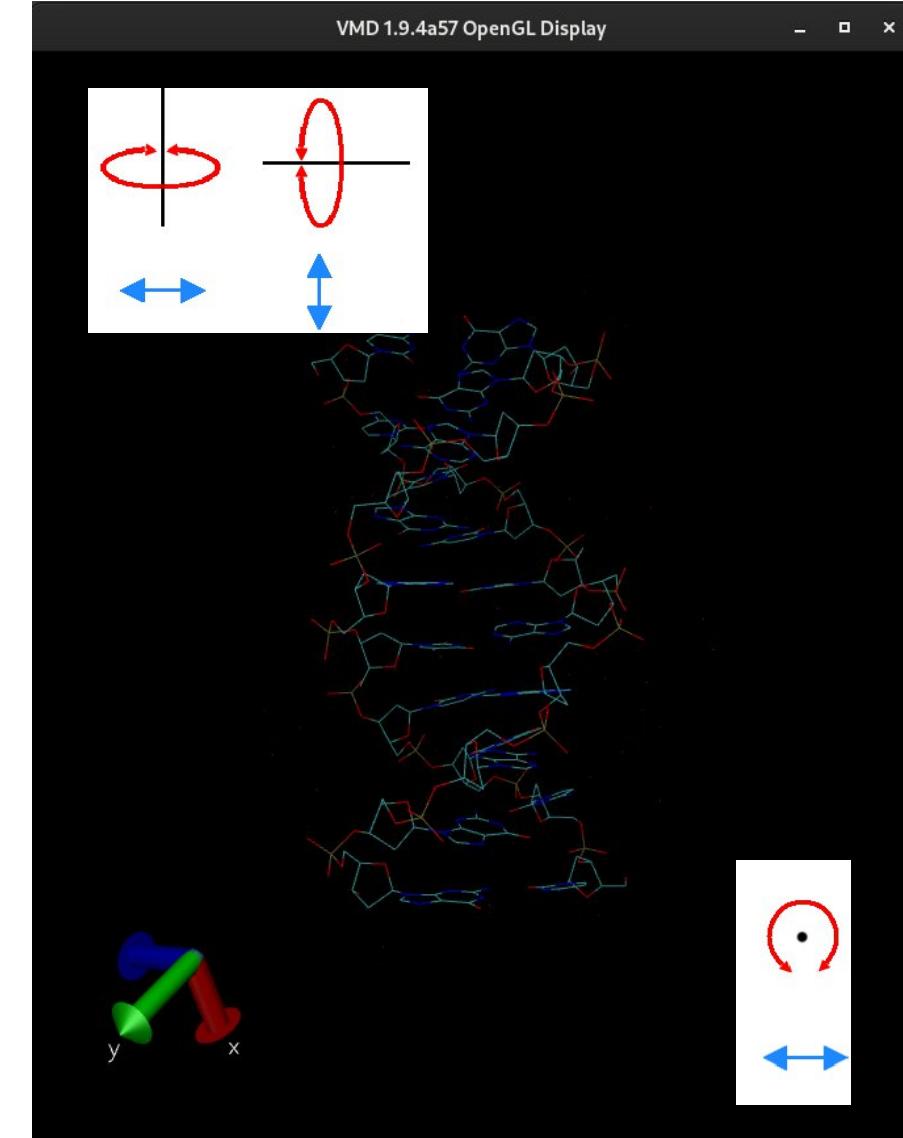
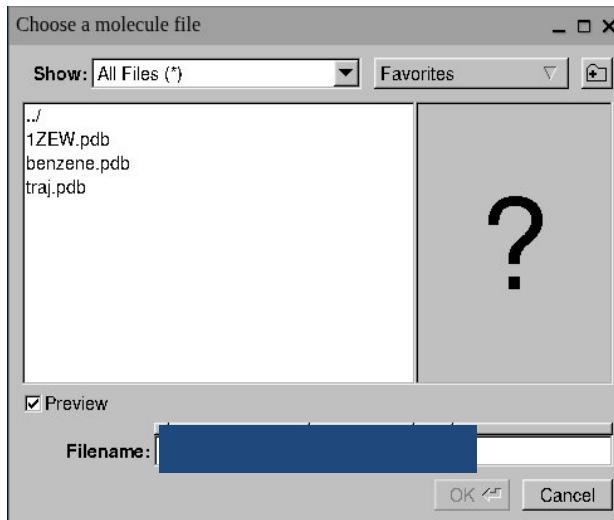
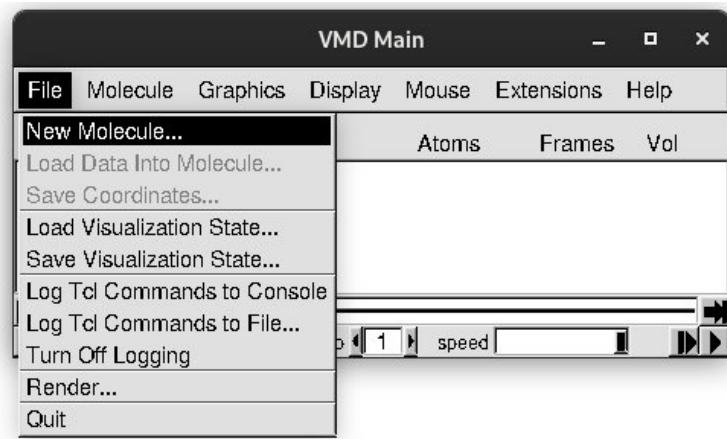
Volumetric Datasets

Automatically  
(Animated) XCrySDen Structure File  
ABINIT  
AMBER Coordinates  
AMBER Coordinates with Periodic Box  
AMBER Parm  
AMBER7 Parm  
AMBER7 Restart  
AVS Field  
Amira File Format (.am)  
Autodock Grid Map  
BRIX Density Map  
Basis Set  
Biomocca Volumetric Map  
CCP4, MRC Density Map  
CHARMM Coordinates  
CHARMM PBEQ Binary Potential Map  
CHARMM,NAMD,XPLOR DCD Trajectory  
CHARMM,NAMD,XPLOR PSF  
CPMD  
DESRES Molecular Structure  
DESRES Trajectory  
DL\_POLY CONFIG  
DL\_POLY\_4 HISTORY  
DL\_POLY\_C HISTORY  
DSN6  
DX  
Delphi 'Big' Formatted Potential Map  
FS4 Density Map  
GAMESS  
GRASP  
GRASP,Delphi Binary Potential Map  
GRID,UHBD Binary Potential Map  
Gaussian Cube  
Gromacs GRO  
Gromacs TRJ Trajectory  
Gromacs TRR Trajectory  
Gromacs XTC Compressed Trajectory  
Gromacs g96  
HOOMD-blue XML File  
InsightII MDF  
InsightII car

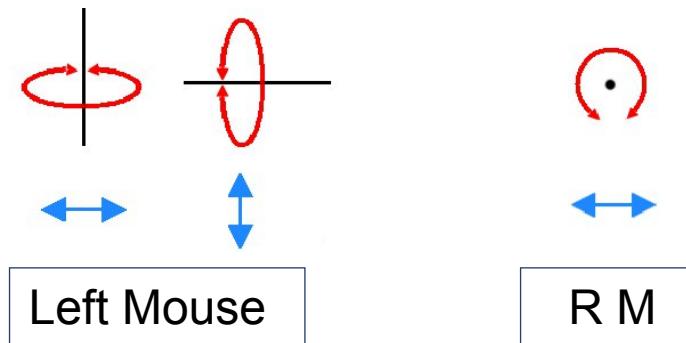
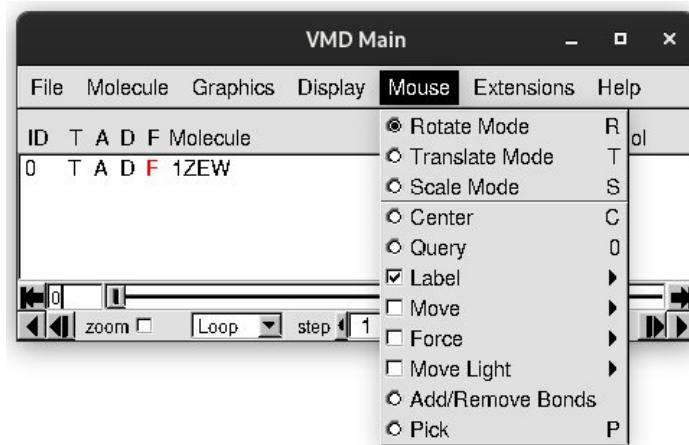
HOOMD-blue XML File  
InsightII MDF  
InsightII car  
Internal Paratool Format  
LAMMPS Trajectory  
Lattice Microbes (RDME)  
MDL mol2  
MSI Biograf Format  
MSMS Surface Mesh  
Maestro File  
Molden  
NAMD Binary Coordinates  
NetCDF (AMBER, MMTK)  
Object File Format (OFF)  
Orca  
**PDB**  
PLY  
PQR  
QCSchema  
Raster3d Scene File  
SPIDER Density Map  
STL Stereolithography Triangle Mesh  
Scripps Binpos  
Situs Density Map  
Tinker  
UHBD Grid  
VASP\_CHGCAR  
VASP\_OUTCAR  
VASP\_PARCHG  
VASP\_POSCAR  
VASP\_XDATCAR  
VASP\_XDATCAR5  
VASP\_xml  
VTF coordinate format  
VTF structure format  
VTF trajectory format  
VTK grid reader  
Web PDB Download  
XPLOR Electron Density Map  
XYZ  
gOpenmol plt  
js  
mmCIF  
polygon mesh  
Convert from:

# Interacting with molecule

/course\_data/git-repo/Day2/01\_VMD/data/1ZEW.pdb

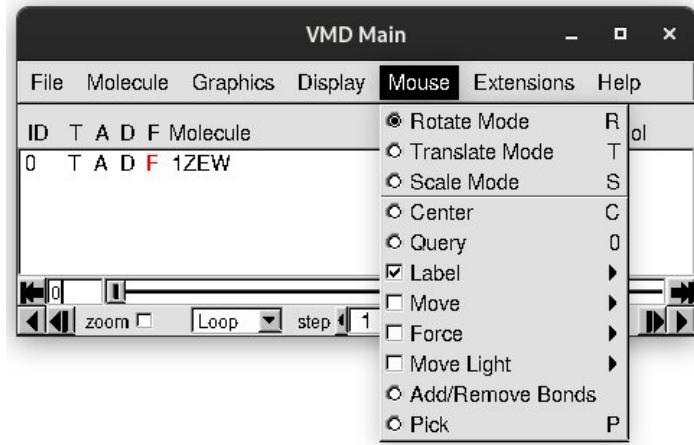


Rotate, translate and scale



# Interacting with molecule

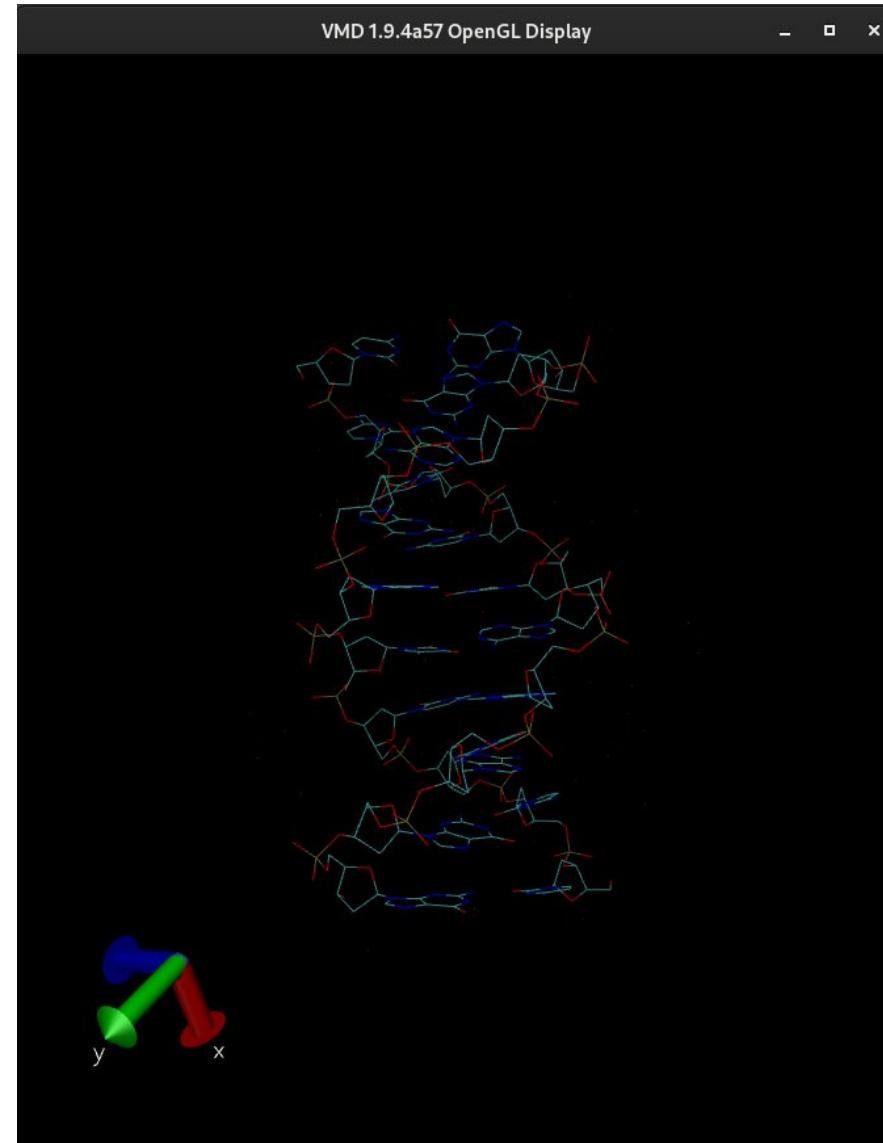
Translate and scale



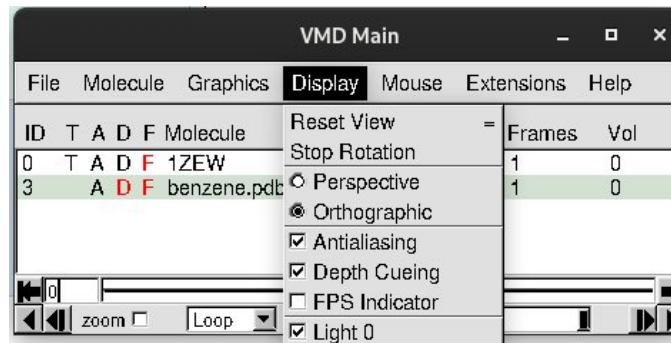
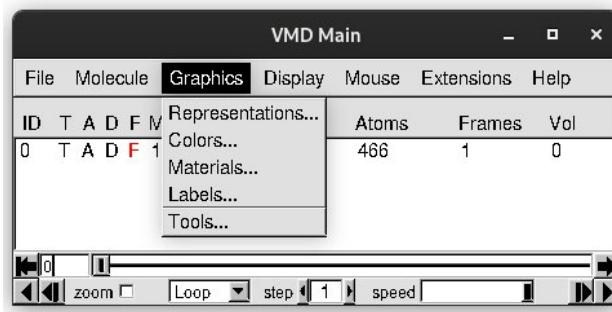
Press T to Translate -



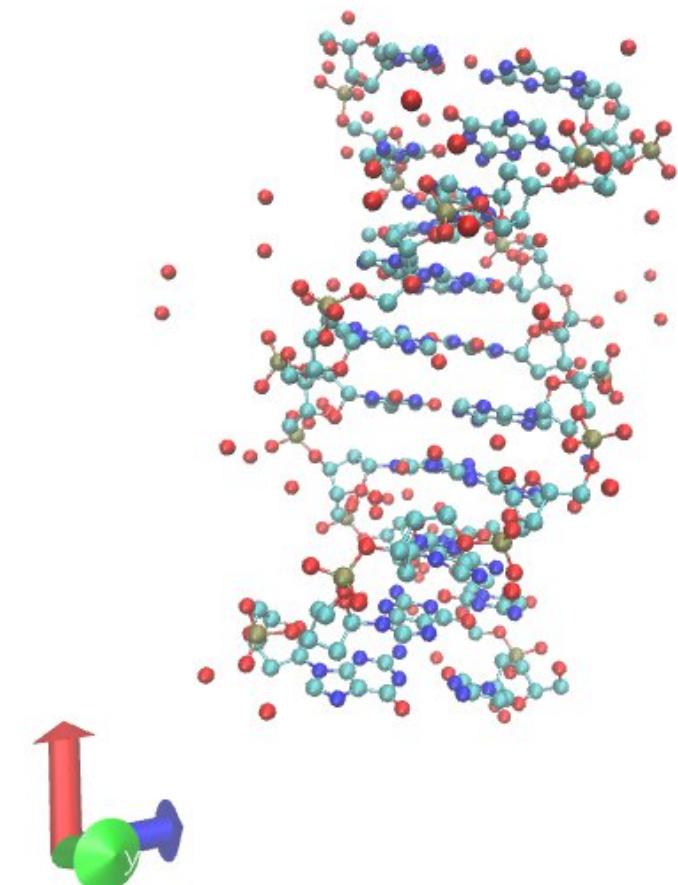
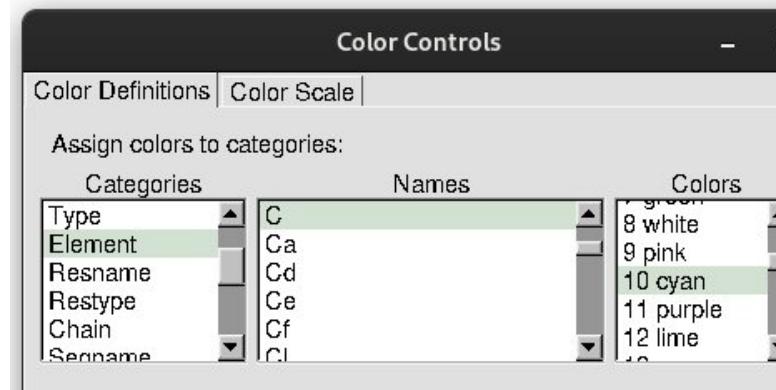
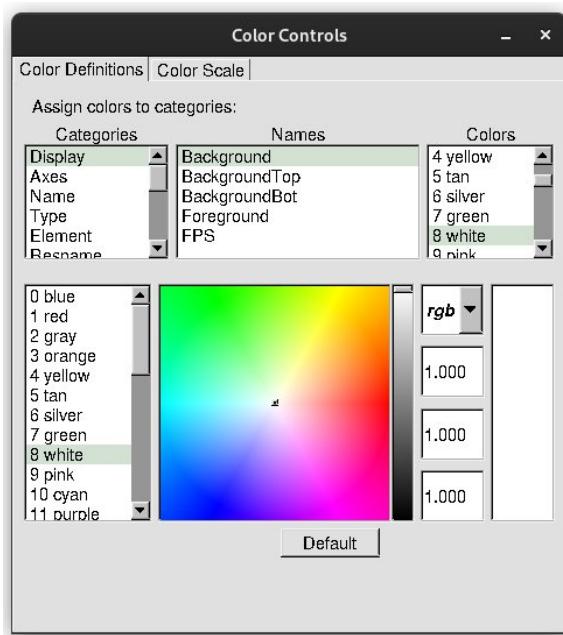
Press S to Scale -



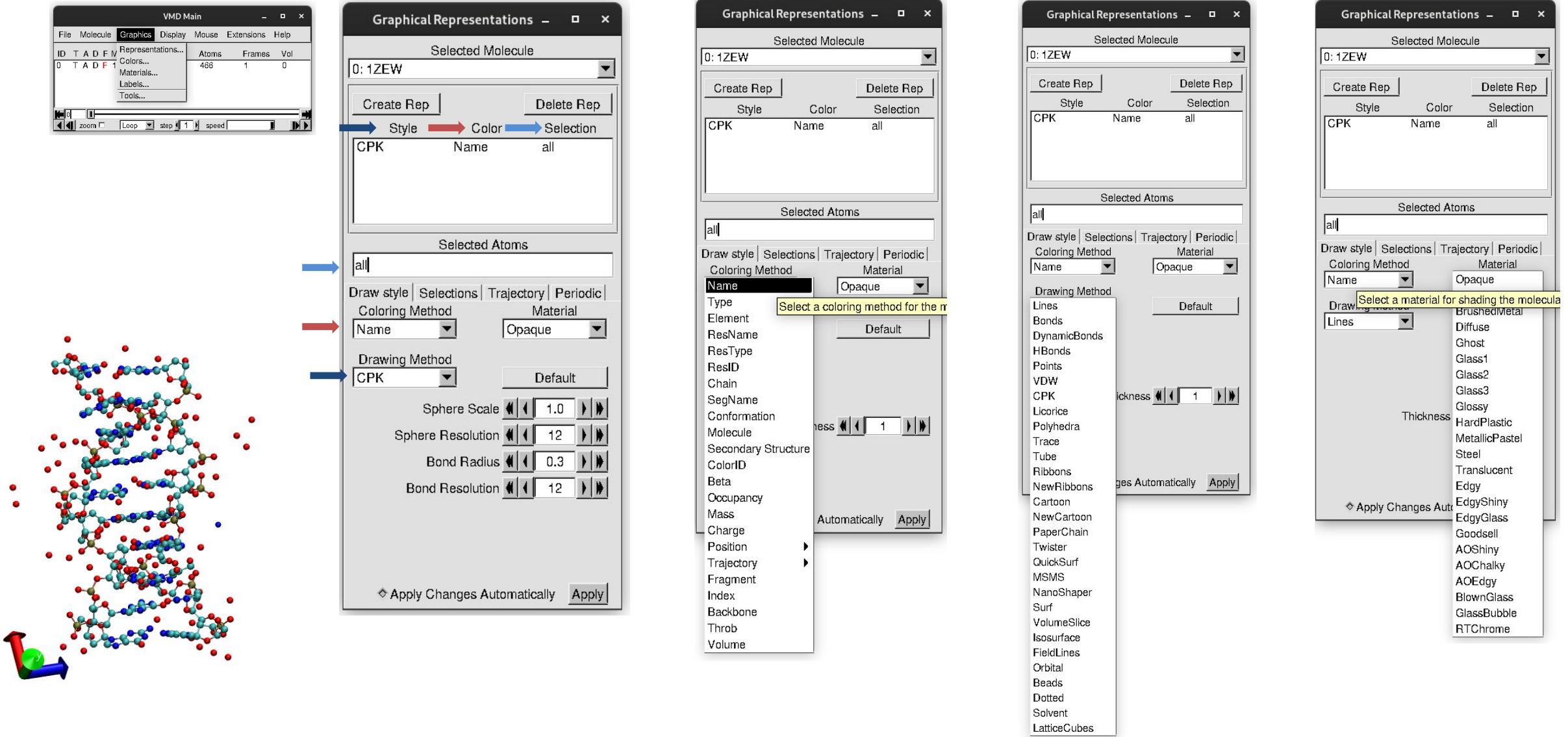
# Color Settings



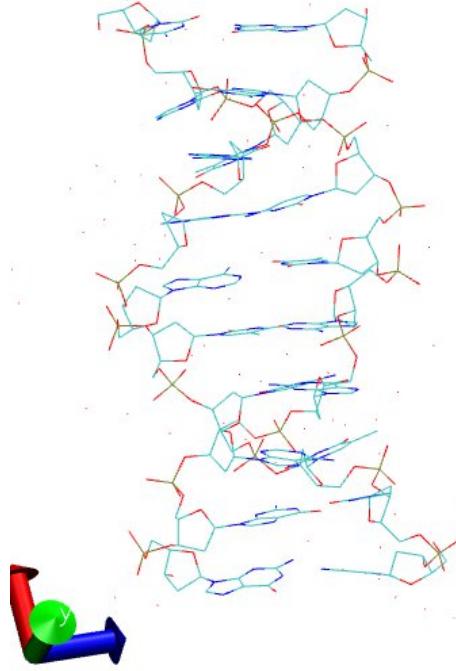
change colors of background, axes, elements....



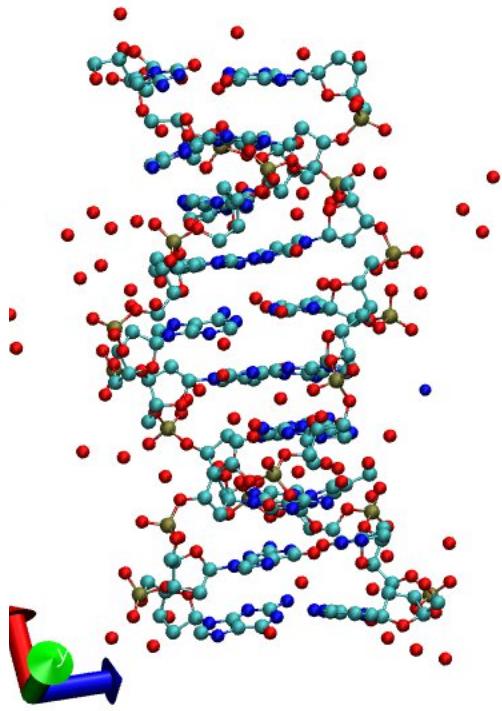
# Graphical Representation



# Graphical Representation: Drawing Method



Lines



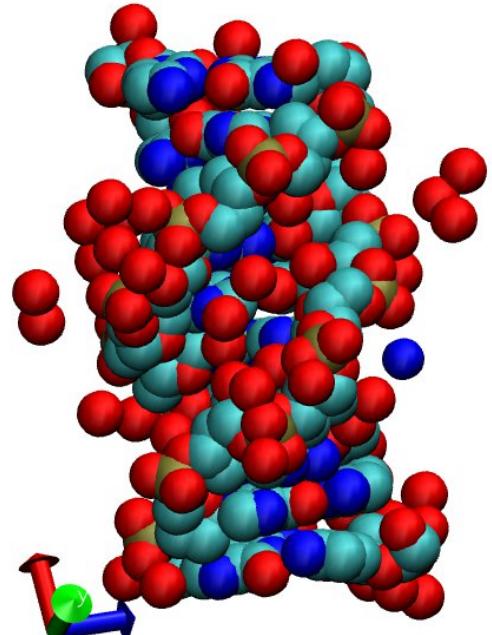
CPK



New Ribbons



New Cartoon



VDW

# Graphical Representation: Selected Atoms

**Graphical Representations -**

Selected Molecule  
0:1ZEW

Create Rep | Delete Rep

Style Color Selection

CPK	Name	all
-----	------	-----

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic |  
Coloring Method | Material

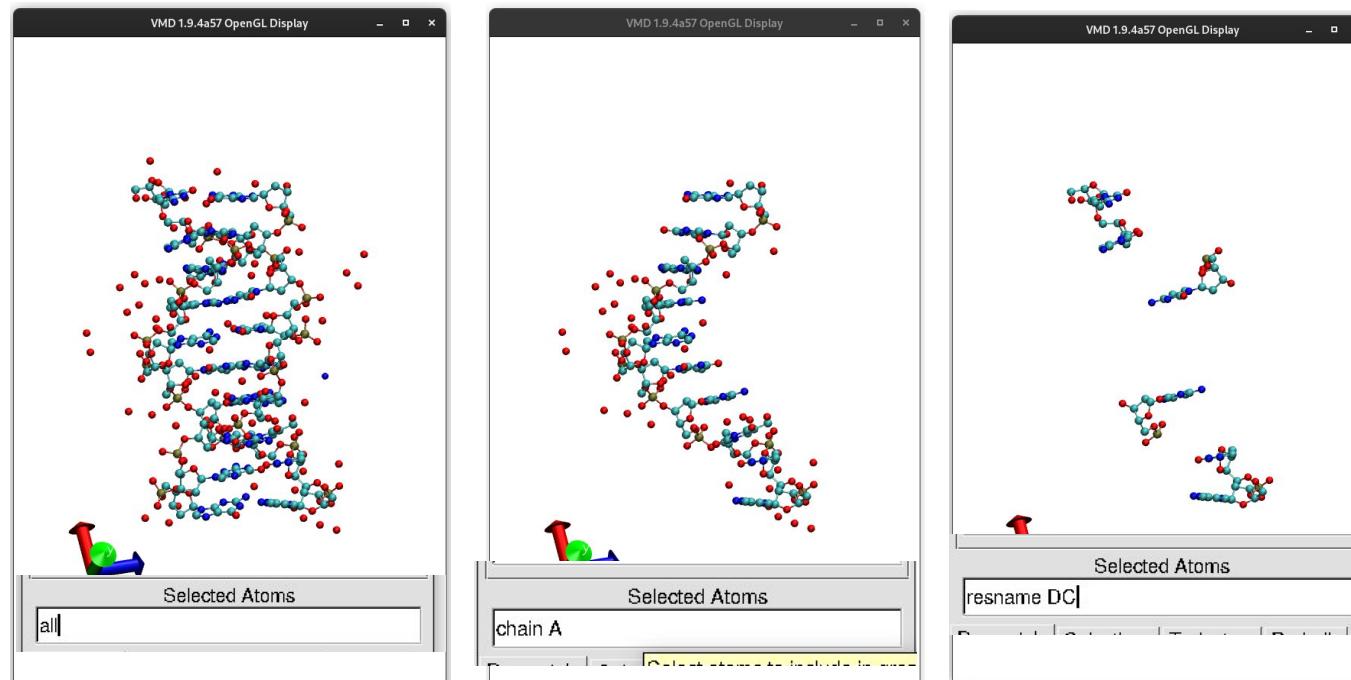
Name	Opaque
------	--------

Drawing Method  
CPK | Default

Sphere Scale | 1.0 |  
Sphere Resolution | 12 |  
Bond Radius | 0.3 |  
Bond Resolution | 12 |

Apply Changes Automatically | Apply

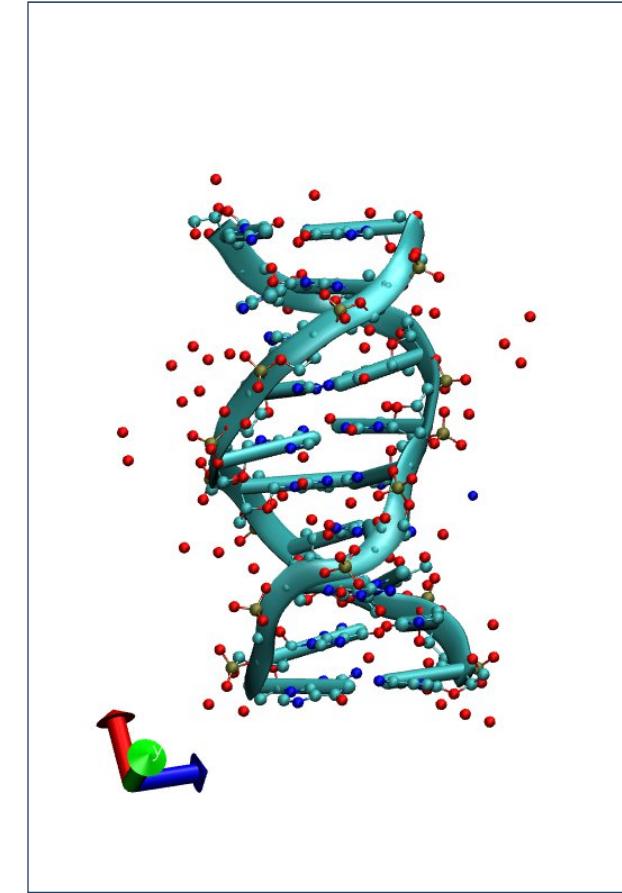
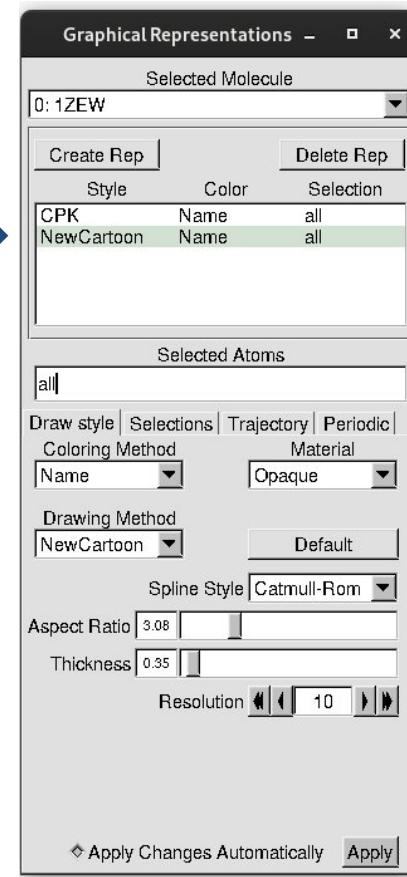
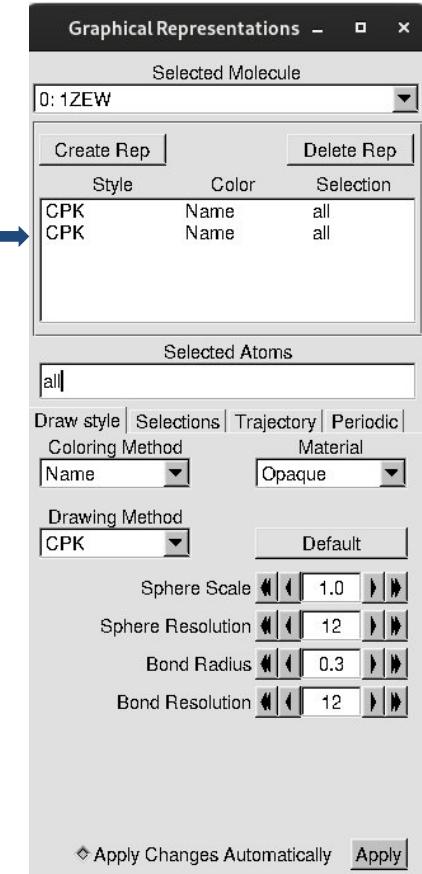
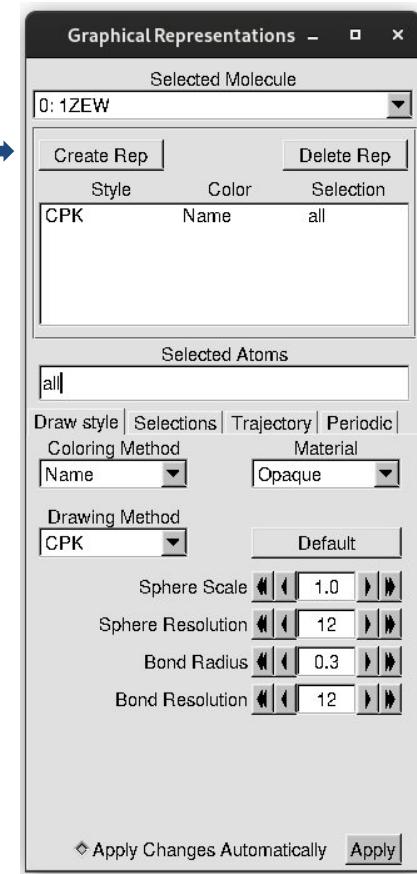
	Serial	type	res	chain	coordinates						
ATOM	1	O5'	DC	A	1	-0.633	0.238	32.103	1.00	23.11	0
ATOM	2	C5'	DC	A	1	-1.560	-0.576	32.829	1.00	22.85	C
ATOM	3	C4'	DC	A	1	-1.619	-1.987	32.293	1.00	22.73	C
ATOM	4	O4'	DC	A	1	-2.109	-1.980	30.932	1.00	PDB File	0
ATOM	5	C3'	DC	A	1	-0.282	-2.719	32.253	1.00	22.77	C



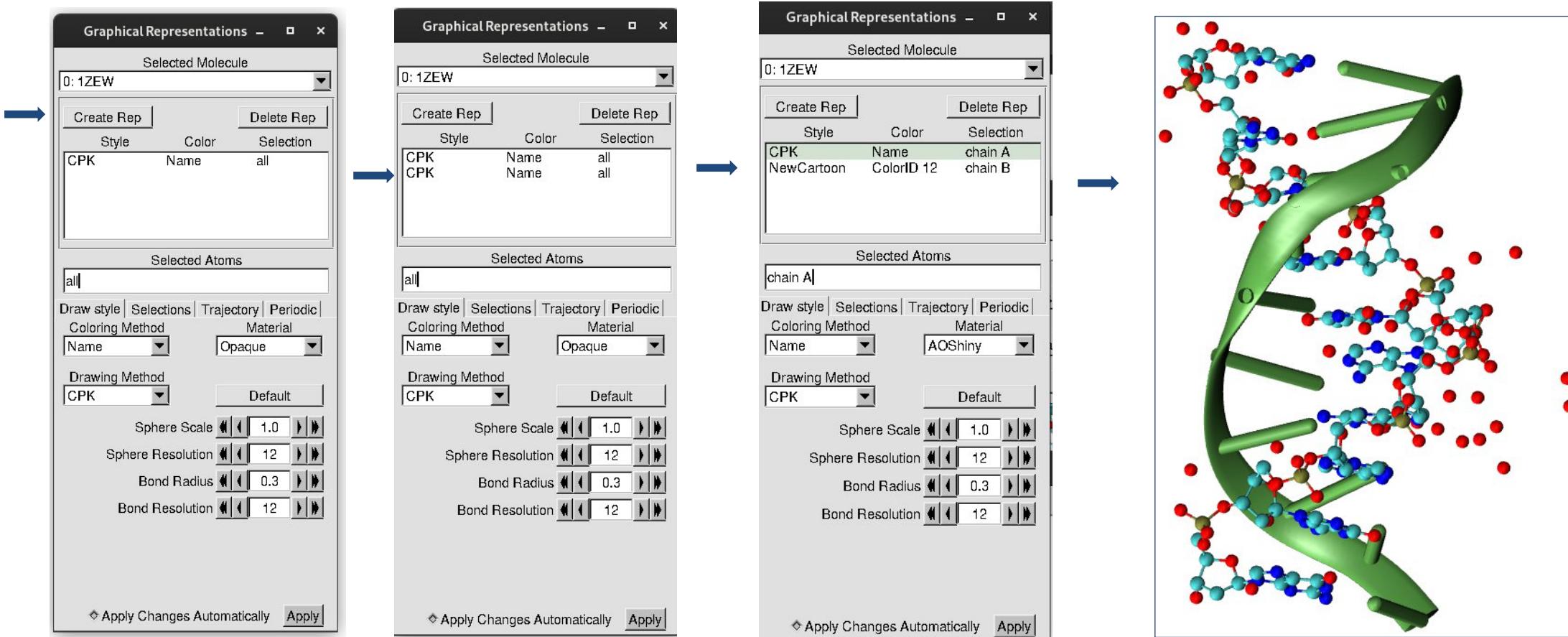
Columns	Data
1-4	"ATOM"
7-11#	Atom serial number
13-16	Atom name
17	Alternate location indicator
18-20\$	Residue name
22	Chain identifier
23-26	Residue sequence number
27	Code for insertions of residues
31-38	X orthogonal Å coordinate
39-46	Y orthogonal Å coordinate
47-54	Z orthogonal Å coordinate
55-60	Occupancy
61-66	Temperature factor
73-76	Segment identifier¶
77-78	Element symbol
79-80	Charge

- index 1- 100
- resname DC
- chain A
- x > 10
- y < 20
- x > 10 && y < 20
- element C
- type O5'
- water

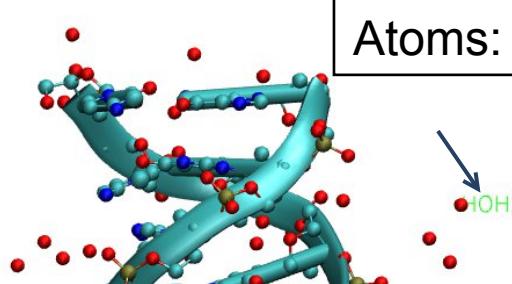
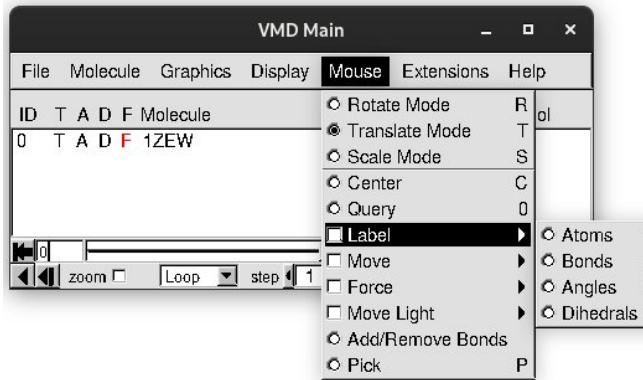
# Graphical Representation: Create Rep



# Graphical Representation: Create Rep



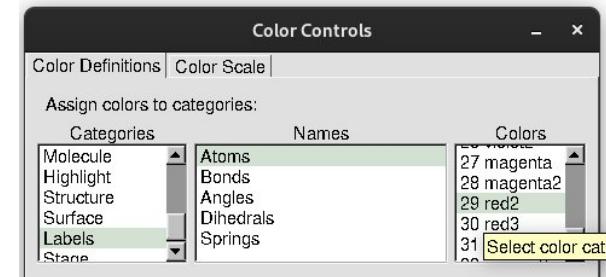
# Label: Atoms, Bonds, Angles and Dihedrals



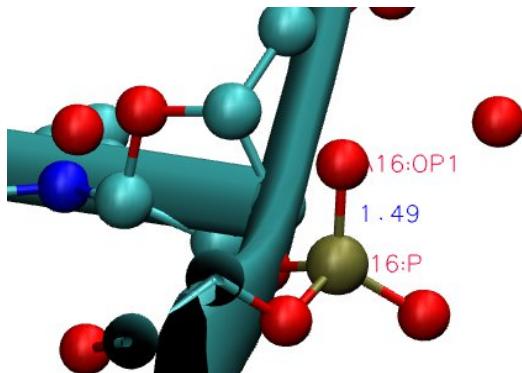
Atoms: 1

```
Info) picked atom:
Info) -----
Info) molecule id: 0
Info) trajectory frame: 0
Info) name: 0
Info) type: 0
Info) index: 436
Info) residue: 52
Info) resname: HOH
Info) resid: 72
Info) chain: A
Info) segname:
Info) x: 18.999001
Info) y: 15.632000
Info) z: 13.699000
Info) Added new Atoms label HOH72:0
```

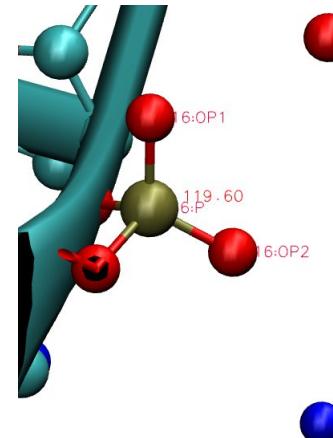
change colors



Bonds: 2

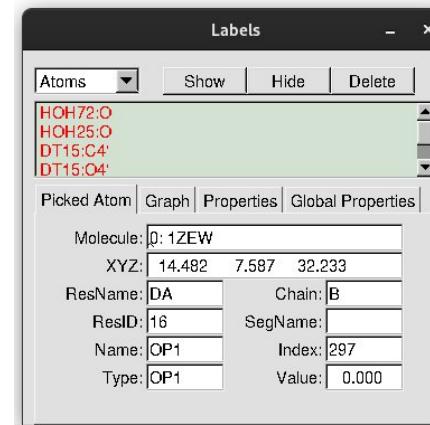


Angles: 3



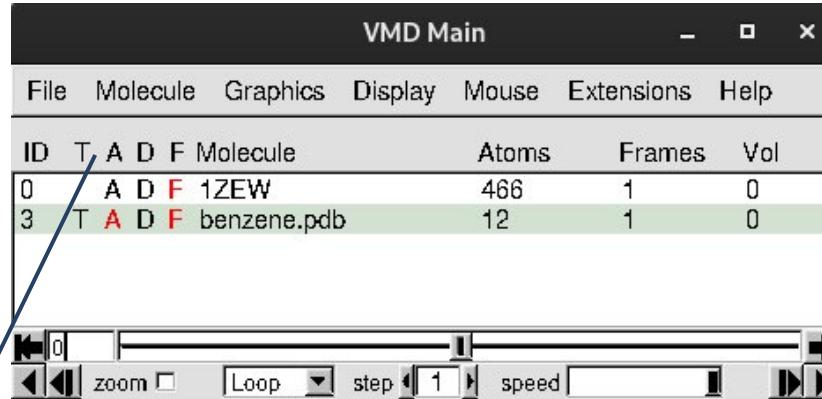
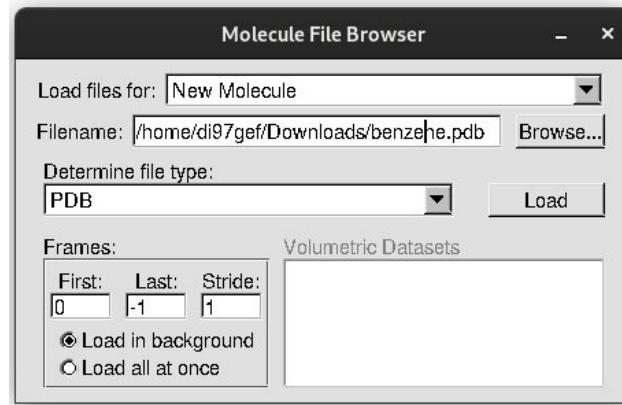
Delete Labels

Graphics > Labels



# VMD Main: Multiple Molecules

Load new molecule



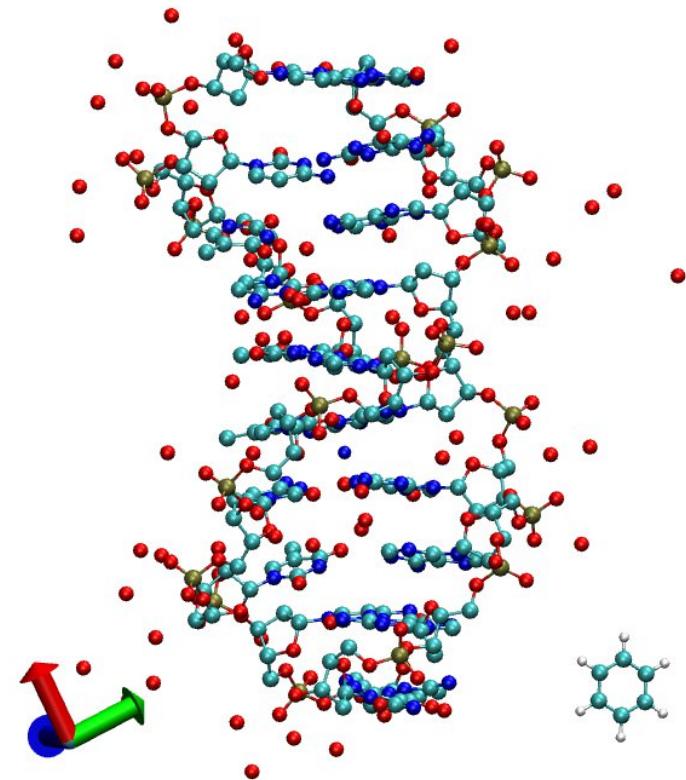
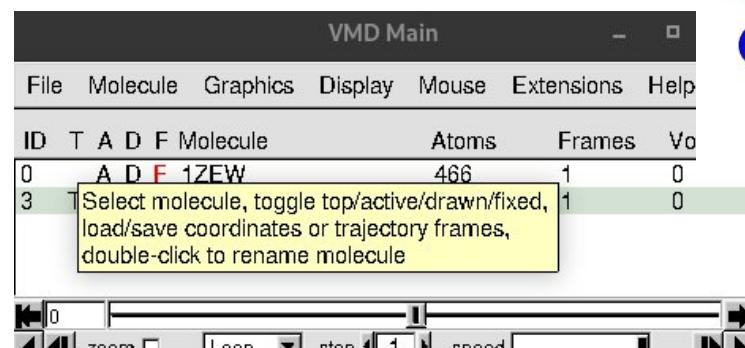
ID - Internal Molecule ID

T - Top; All actions apply to top molecule

A - Active; Trajectory update status

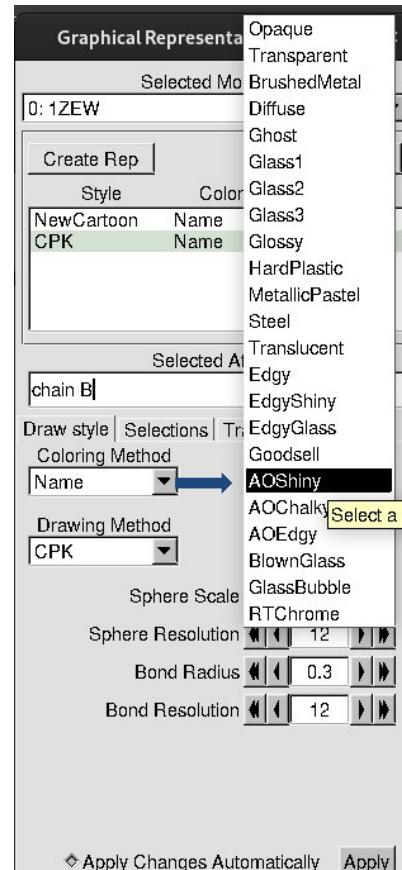
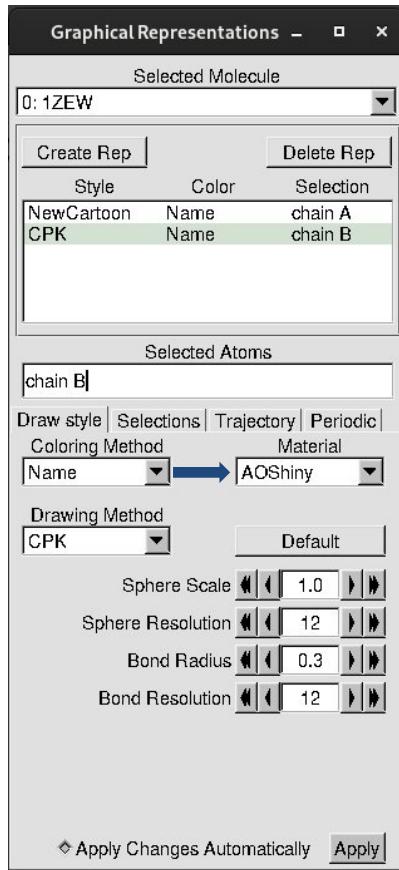
D - Drawn

F - Fixed

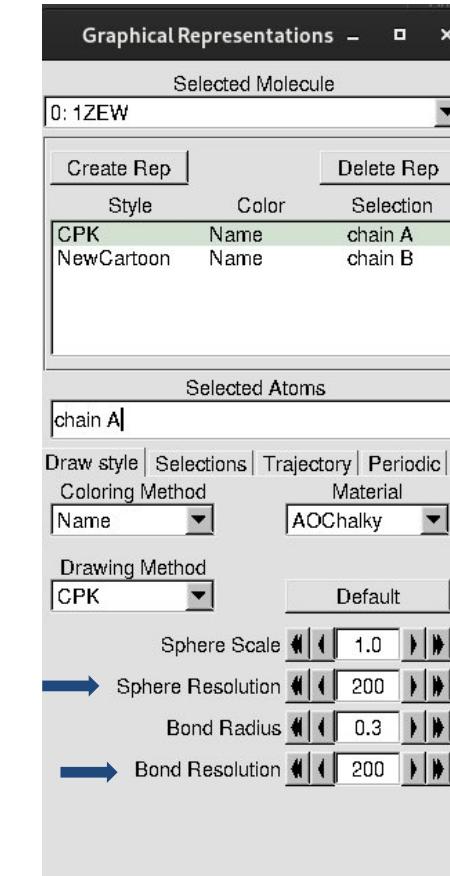
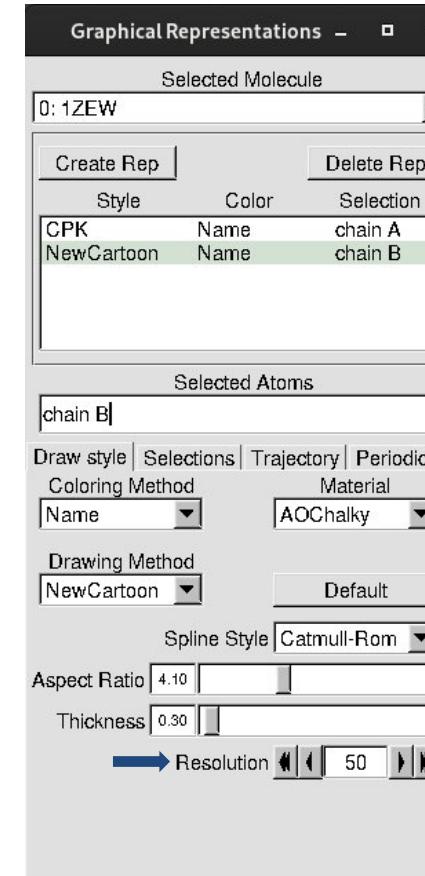


# Rendering: Publication Quality Images

## Change Material Type

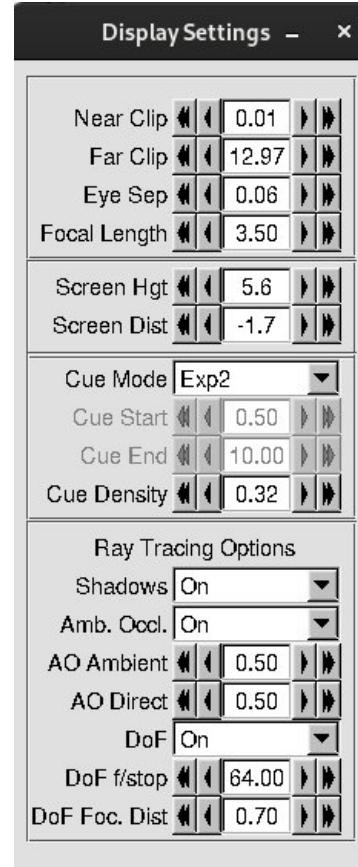
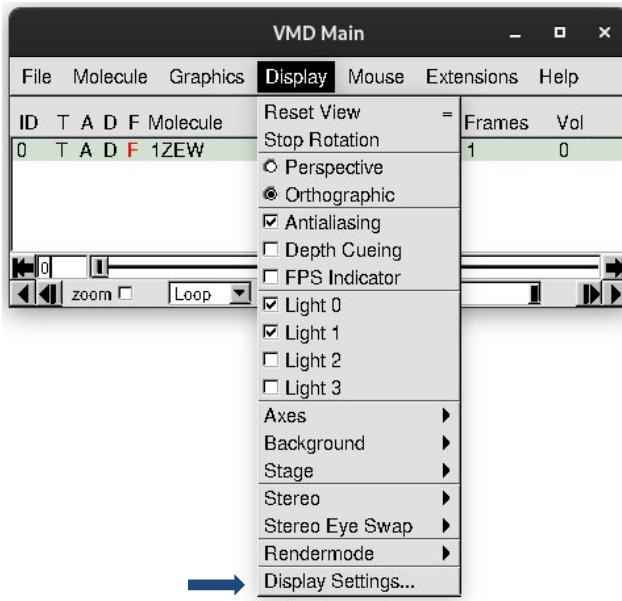


## Change Resolution

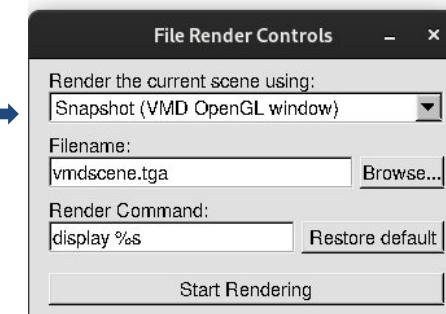
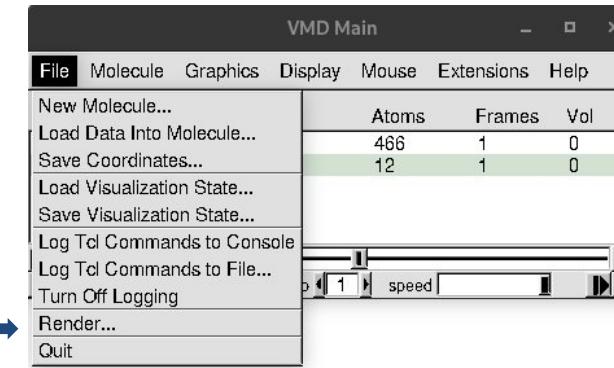


# Rendering: Publication Quality Images

Go to Display Settings



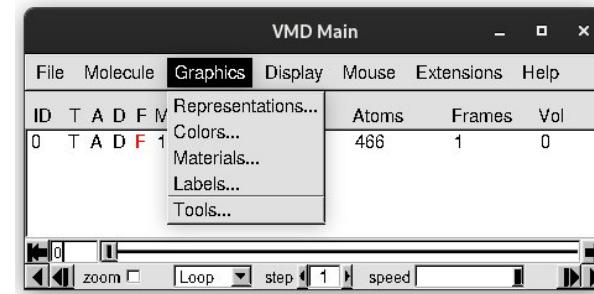
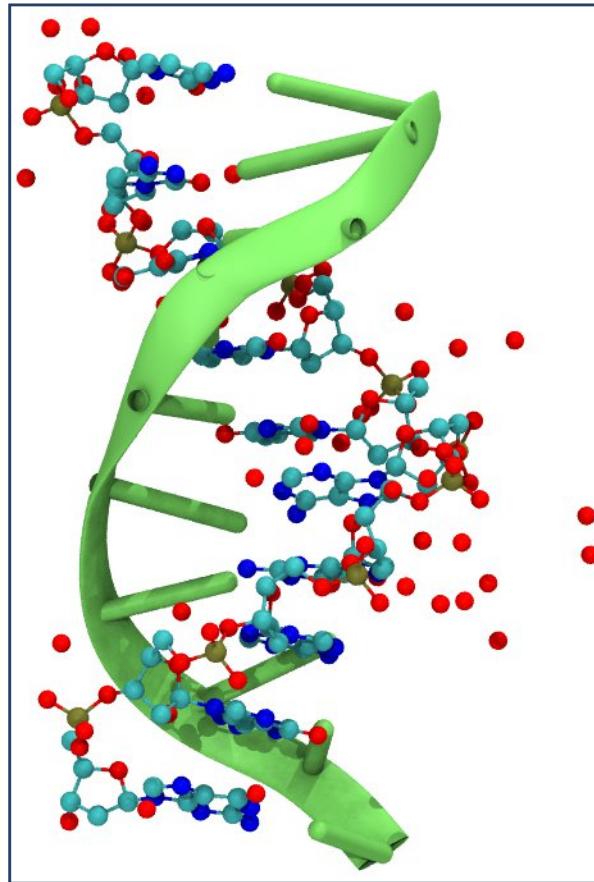
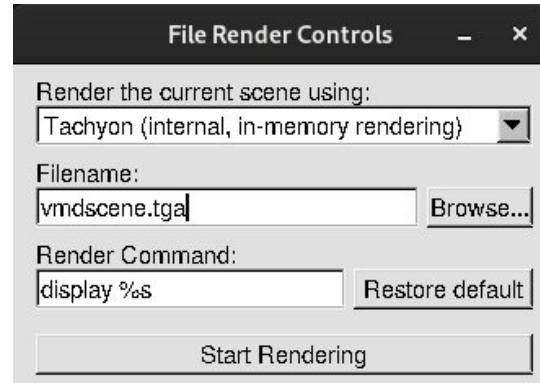
Go to render settings



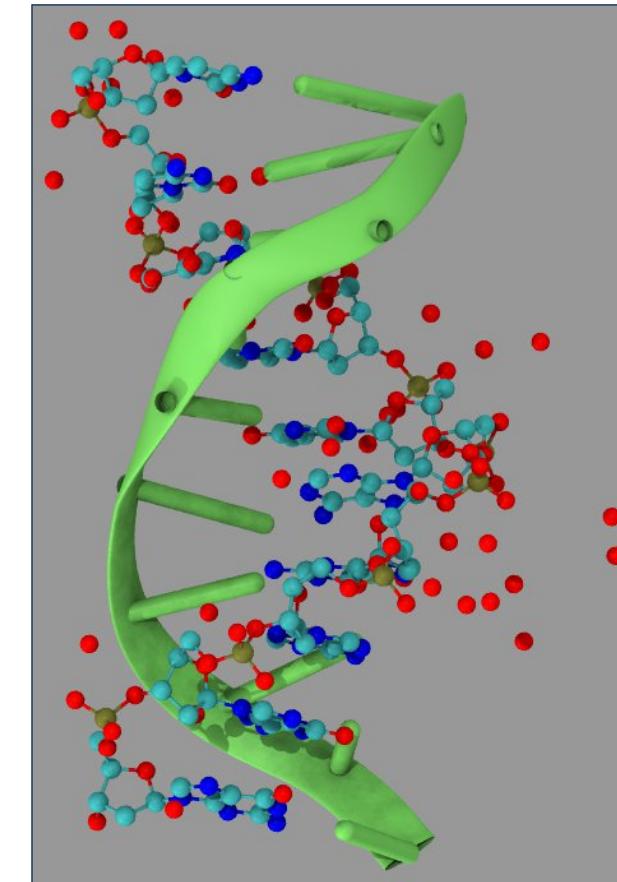
- ART (VORT ray tracer)
- NVIDIA Gelato 2.1
- PostScript (vector graphics)
- Raster3D 2.7d
- Radiance 4.0
- Rayshade 4.0
- PIXAR RenderMan
- Snapshot (VMD OpenGL window)
- STL (triangle mesh only)
- Tachyon
- Tachyon (internal, in-memory rendering)**
- TachyonL-OSPRay (internal, in-memory, SSE+AVX-accelerated)
- TachyonL-OSPRay (interactive, SSE+AVX-accelerated)
- POV-Ray 3.6
- VRML 1.0 (VRML94)
- VRML 2.0 (VRML97)
- Wavefront (OBJ and MTL)
- X3D (XML) full specification
- X3D (XML) limited subset for X3DOM v1.1

# Rendering: Publication Quality Images

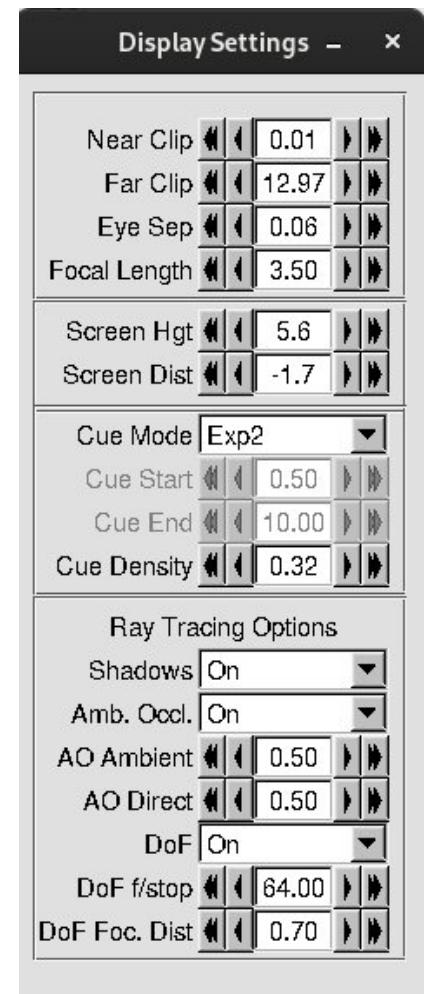
## Render Image



color > background > grey

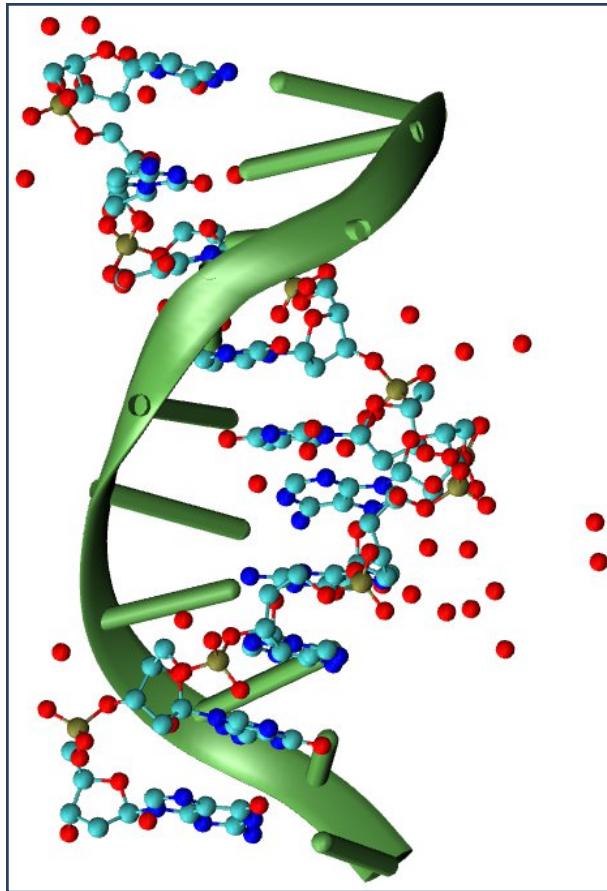


Fine tune Settings

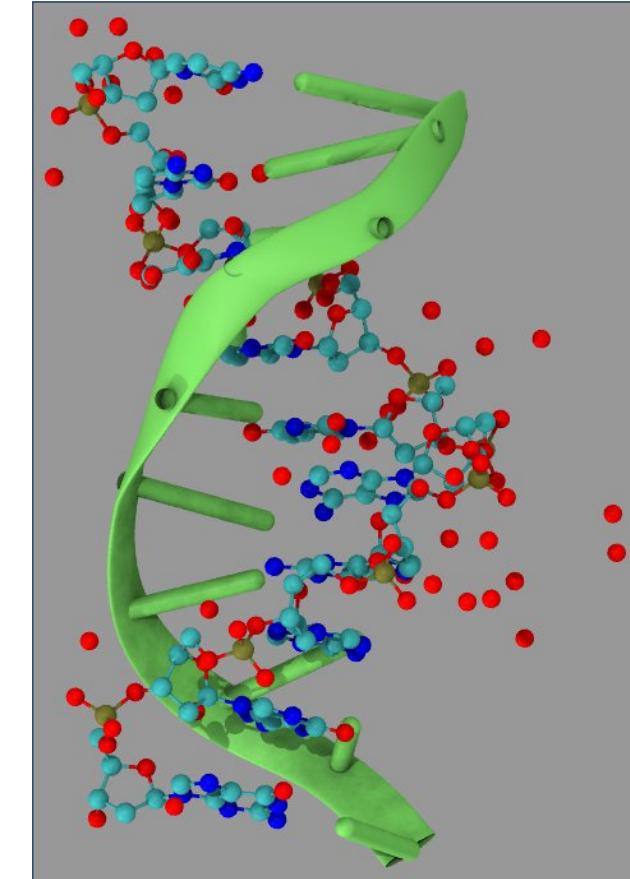
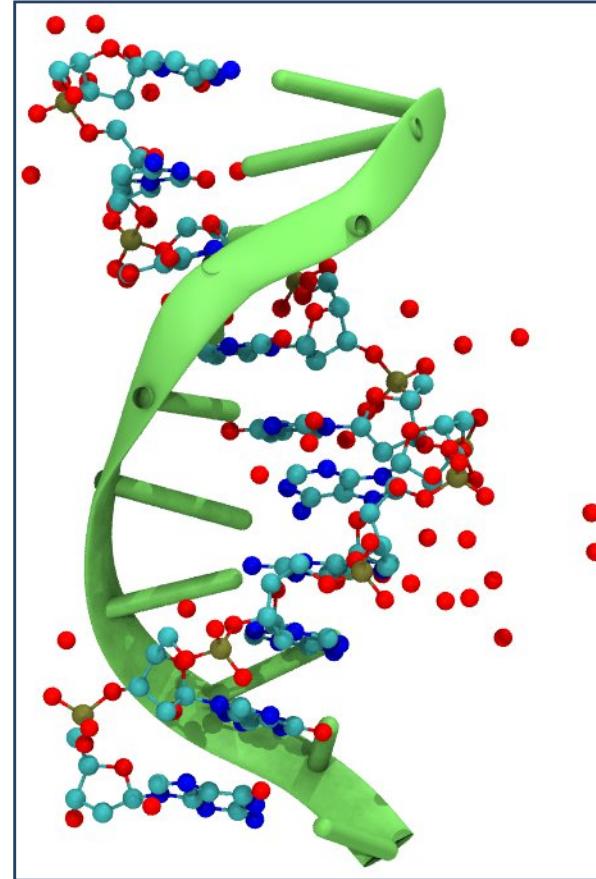


# Rendering: Publication Quality Images

Using VMD Snapshot

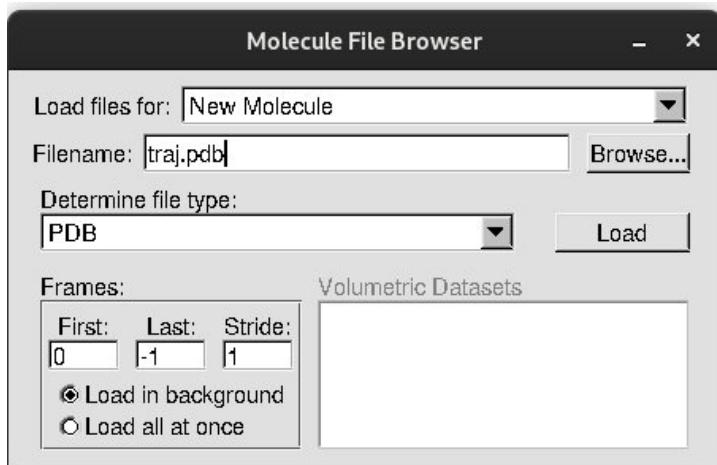


Using Tachyon Internal



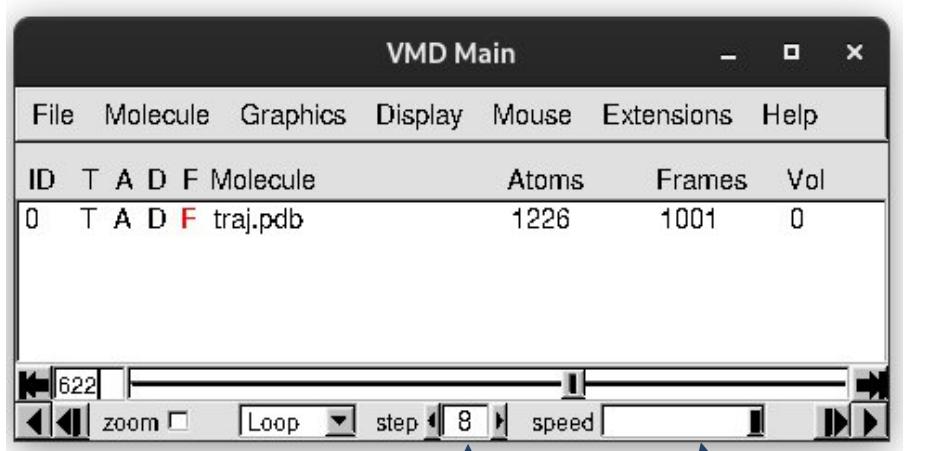
# VMD: Loading Trajectories

Load trajectory



Load custom Frames

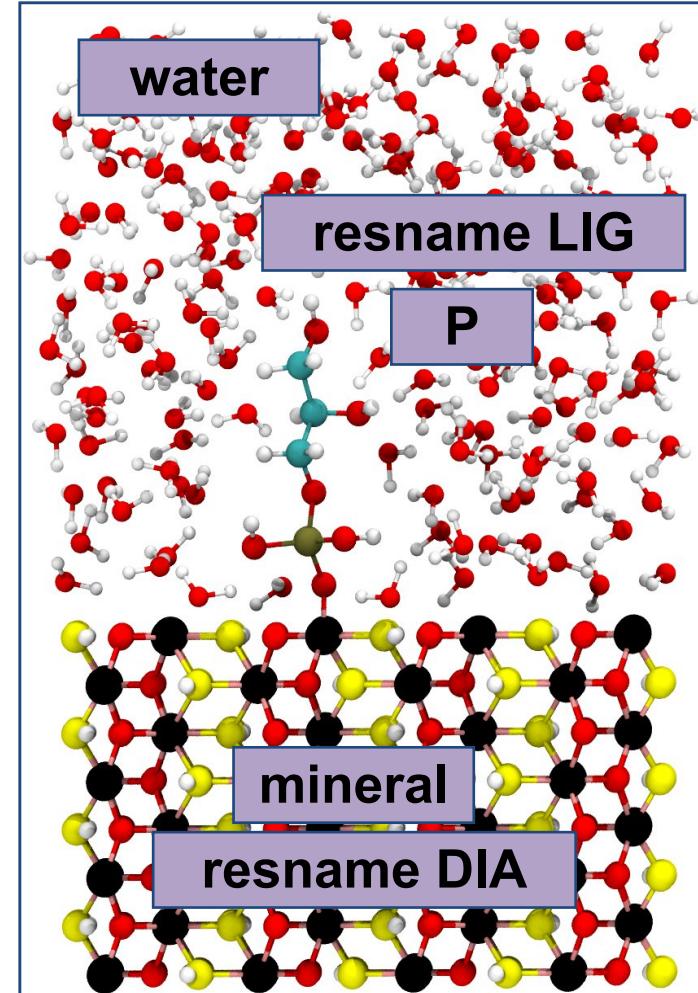
/custom\_software/course\_data/vmd



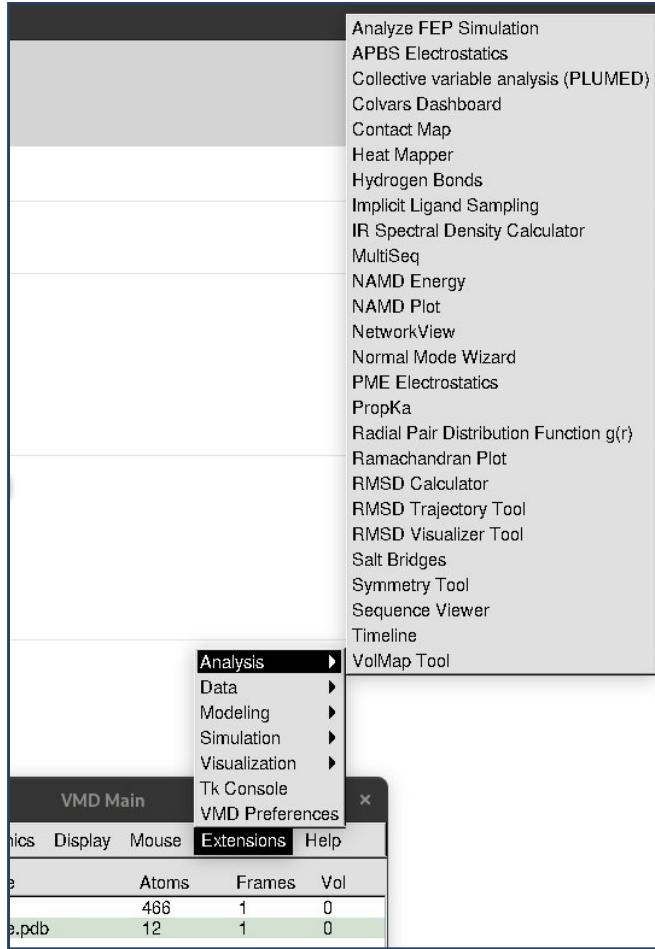
Loop/rock

show every 8th step

Speed of frames



# VMD: Trajectory Analysis



Hydrogen Bond Analysis

Radial Pair Distribution Function

RMSD

# VMD: Trajectory Analysis

## Hydrogen Bond Analysis

Hydrogen Bonds

Input options

Molecule: 0: traj.pdb

Selection 1 (Required): resname LIG

Selection 2 (Optional): water

NOTE: if sel1 and sel2 overlap, hbonds output is unreliable!

Frames: all (now, all, b:c, or b:c:e)

Update selections every frame?  Only polar atoms (N, O, S, F)?

Selection 1 is the:  Donor  Acceptor  Both

Donor-Acceptor distance (Å): 3.0

Angle cutoff (degrees): 40

Calculate detailed info for:  None  All hbonds  Residue pairs  Unique hbond

Output options

Plot the data with MultiPlot?

Output directory: /home/di97gef/Documents/lrz/work/biophy\_ec

Log file?

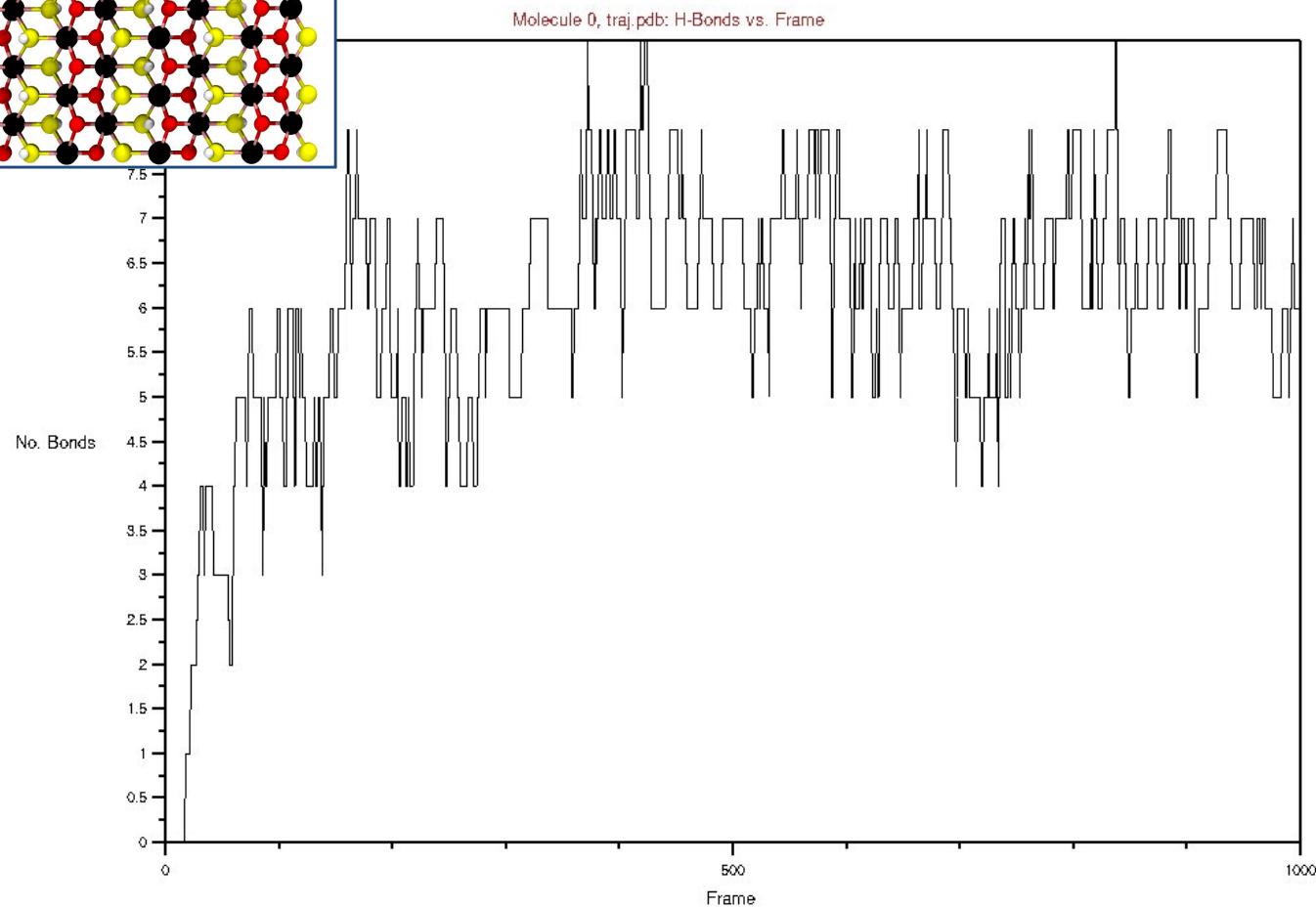
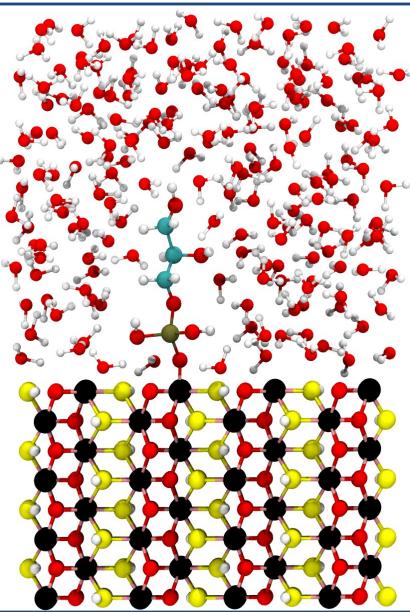
Write output to files?

Frame/bond data? hbonds.dat

Detailed hbond data? hbonds-details.dat

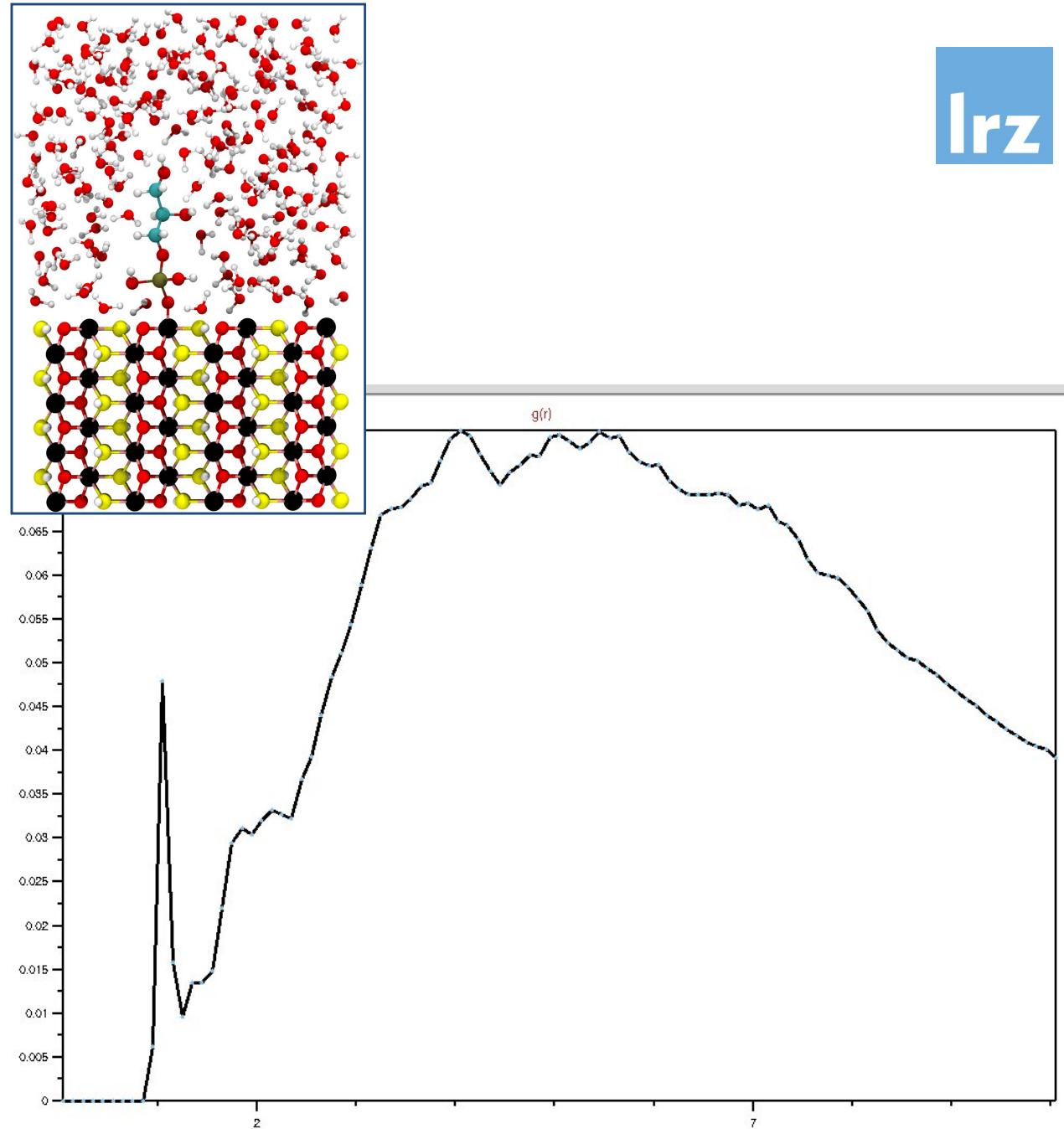
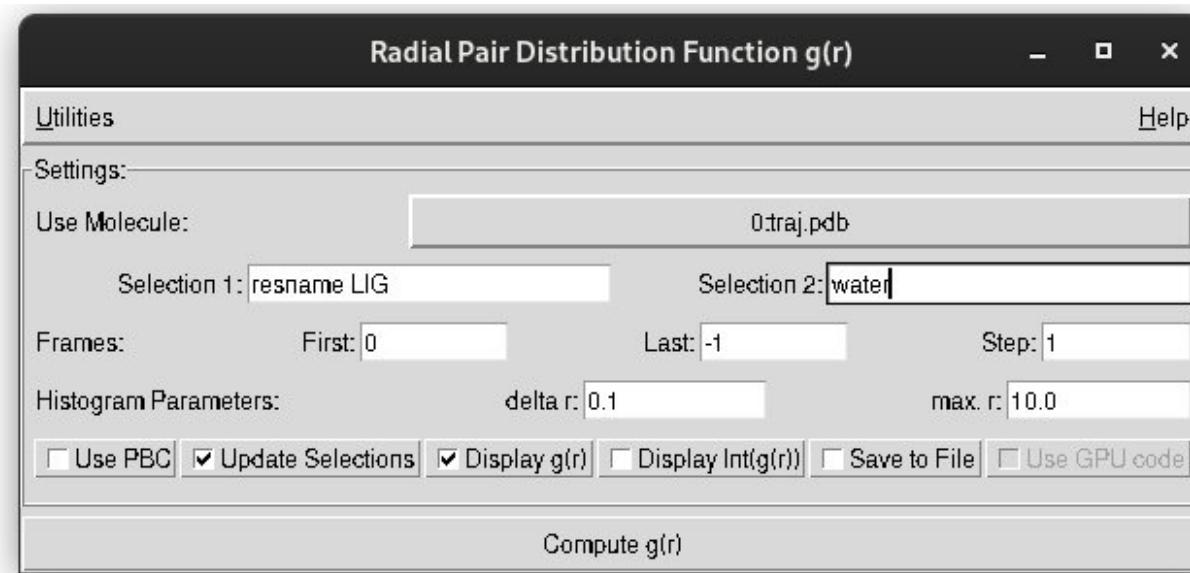
Status

Ready.



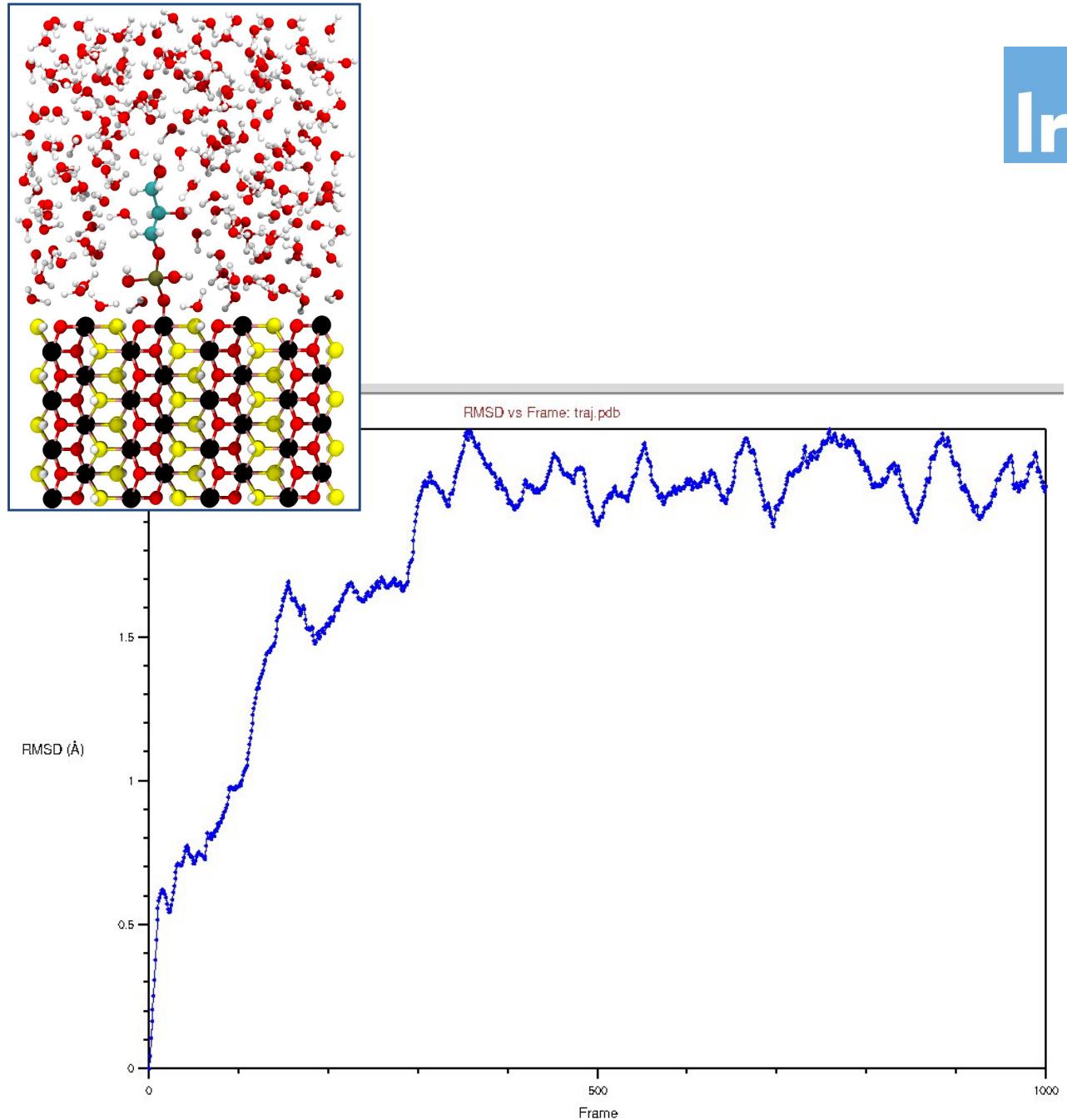
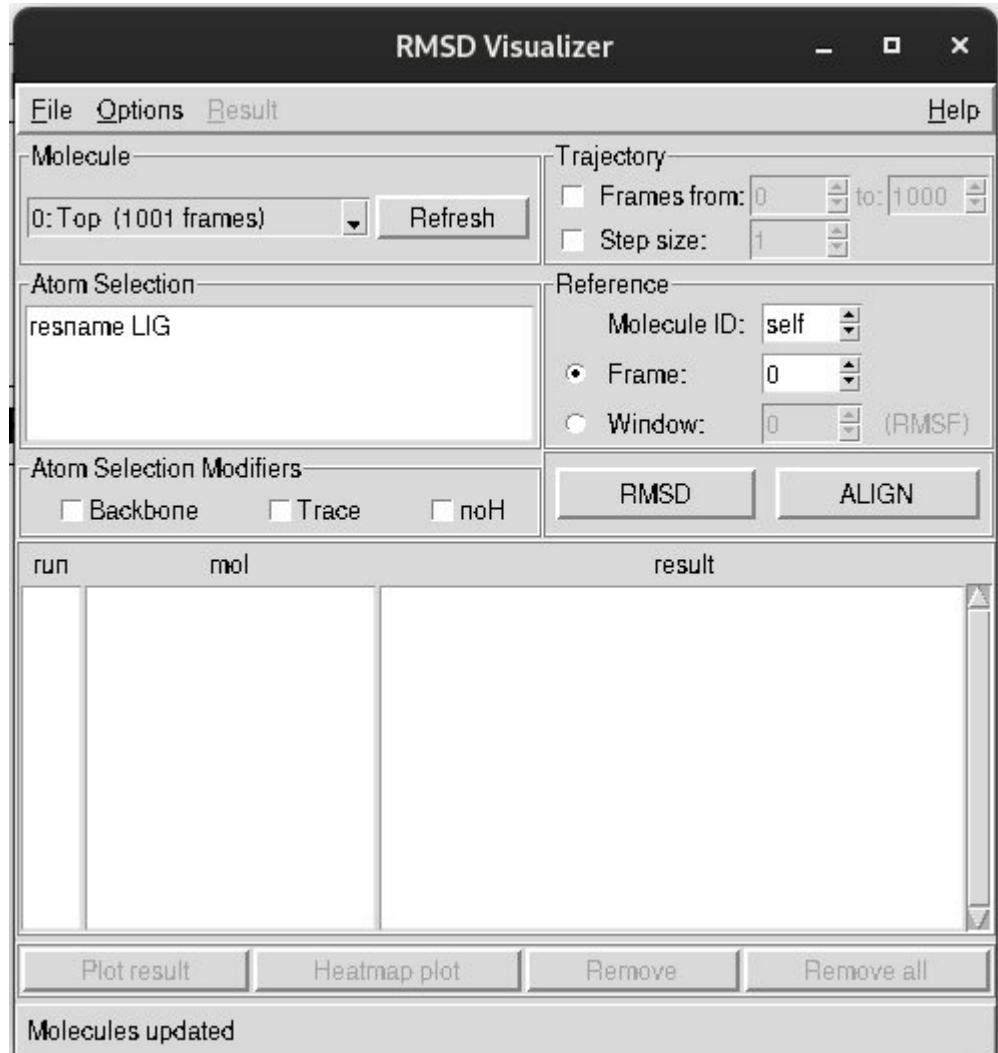
# VMD: Trajectory Analysis

## Radial Pair Distribution Function



# VMD: Trajectory Analysis

## RMSD Visualizer Tool



# VMD: Summary

- Visualizes molecular structures (proteins, DNA, membranes)
- Displays MD trajectories
- Supports multiple formats: **PDB, PSF, DCD, GRO, XTC, etc**
- Advanced rendering: cartoon, licorice, surface, VDW
- Plugins for analysis (RMSD, hydrogen bonds)

Advanced:

- Supports **Tcl and Python scripting** for automation
- <http://www.ks.uiuc.edu/Training/Tutorials/#vmd>

