



# Introduction to VMD

*Using the GUI effectively*

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Systems, Synthetic, and Physical Biology Ph.D. Program

# Agenda



Installing VMD



Basic UI  
elements



Rendering  
images



Rendering  
videos

# Visual Molecular Dynamics, VMD



## VMD Website

NIH RESOURCE FOR MACROMOLECULAR MODELING & VISUALIZATION | UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

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**VMD**  
Visual Molecular Dynamics

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.  
[\(more details...\)](#)

**Spotlight**

In 2017, the Royal Swedish Academy of Sciences awarded the Nobel Prize in Chemistry to Jacques Dubochet, Joachim Frank, and Richard Henderson "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution". We are pleased to celebrate this great triumph for structural biology along with the well-deserved recognition of the Center's long-time collaborator and friend, Joachim Frank. Our center has a long tradition in developing computational methods that enable scientists to build atomistic models of biomolecules. Molecular Dynamics Flexible Fitting (MDFF), a method developed in close collaboration with Joachim Frank and his group, reconciles high resolution data from X-ray crystallography and functional information from cryo-electron microscopy (cryo-EM). MDFF utilizes molecular dynamics to "naturally" fit each atom into a cryo-EM map. In less than a decade since its development, MDFF has proved instrumental in studying biomolecular systems. A selected list of publications employing MDFF both by our group and others can be found [here](#).

Other Spotlights

**Overview** **News and Announcements**

Dynamics of chromosome organization in a minimal bacterial cell, FCDB, 2023 NEW  
VMD as a Platform for Interactive Small Molecule Preparation and Visualization in Quantum and Classical Simulations, JCIM, 2023 NEW  
Human Learning for Molecular Simulations: The Collective Variables Dashboard in VMD, JCTC, 2022  
ANARI: A 3D Rendering API Standard, CISE, 2022  
#COVIDisAirborne: AI-Enabled Multiscale Computational Microscopy of Delta SARS-CoV-2 in a Respiratory Aerosol, IJHPCA, 2022  
Intelligent Resolution: Integrating Cryo-EM with AI-Driven Multi-Resolution Simulations to Observe the SARS-CoV-2 Replication-Transcription Machinery in Action, IJHPCA, 2022  
The Coronavirus in a Tiny Drop, VMD visualizations of aerosolized SARS-CoV-2, NYT, 2021  
NIH Director's blog highlights neuroscience adaptation of VMD  
AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics, IJHPCA, 2021  
Multiscale modeling and cinematic visualization of photosynthetic energy conversion processes from electronic to cell scales, J. Par. Comp. 2021  
NAMD and VMD part of the team winning the ACM COVID-19 Gordon Bell Prize for 2020  
The Coronavirus Unveiled, VMD visualizations of SARS-CoV-2, NYT, 2020  
Scalable molecular dynamics on CPU and GPU architectures with NAMD, JCP, 2020  
VMD test builds for MacOS X 10.15 "Catalina" (April 24, 2020)  
Past announcements

**Download**

Download (all versions)  
VMD 2.0.0 alpha (Unix)  
VMD 1.9.4 (MacOS X, Unix, Windows)  
VMD 1.9.3 (MacOS X, Unix, Windows)  
VMD script library  
License, Copyright and Disclaimer

**Gallery**

An Accessible Visual Narrative for the Primary Energy Source of Life from the Fulldome Show Birth of Planet Earth, 1st Place Winner, SC'19 Viz. Showcase

A large black arrow points to the "Download" section of the left sidebar.

# Visual Molecular Dynamics, VMD



## VMD Website

The screenshot shows the "Software Downloads" section of the VMD website. The left sidebar has a "Software" category selected, showing options like NAMD, VMD, GPU Computing, Lattice Microbes, etc. The main content area lists download links for different VMD versions across various platforms. A large bracket on the right side groups the download sections under the heading "Select platform".

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**Software Downloads**

**Download VMD:**

VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. Visit the [VMD website](#) for complete information and documentation.

Selecting an archive below will lead to a user registration and login page. Your download will continue after you have registered or logged in.

**Version 2.0.0 LATEST ALPHA (2025-08-19) Platforms:**

Latest pre-release ALPHA test version

- [LINUX\\_64 \(RHEL 8+\) OpenGL, CUDA, OptiX RTX, RTX RTRT](#) (Linux (RHEL 8+) 64-bit Intel/AMD x86\_64 SSE/AVX+ with CUDA 10, OptiX6.5 RTX, RTX RTRT)
- [MacOS 11.x, ARM64 \(64-bit "M1" Macs\)](#) (Apple MacOS-X 11 or later)
- [Windows 64-bit, CUDA \(64-bit Intel x86\\_64\)](#) (Windows 11)

**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 (RHEL 7+) 64-bit Intel/AMD x86\_64 SSE/AVX+ with CUDA 10, OptiX6.5 RTX, OSPRay)
- [LINUX\\_64 \(RHEL 7+\) OpenGL, CUDA, OptiX RTX, OSPRay, RTX RTRT](#) (Linux (RHEL 7+) 64-bit Intel/AMD x86\_64 SSE/AVX+ with CUDA 10, OptiX6.5 RTX, OSPRay, RTX RTRT)
- [MacOS 11.x, ARM64 \(64-bit "M1" Macs\)](#) (Apple MacOS-X 11 or later)
- [MacOS 10.15, x86\\_64 \(64-bit Intel x86\\_64\)](#) (Apple MacOS-X 10.15 or later)
- [Windows 64-bit, CUDA, OptiX, OSPRay \(64-bit Intel x86\\_64\)](#) (Windows 10)

**Version 1.9.3 (2016-11-30) Platforms:**

We recommend that all users upgrade to VMD 1.9.3

- [Source Code](#)
- [LINUX\\_64 OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 SSE, with CUDA 8.x, OptiX, OSPRay)
- [LINUX\\_64 Text-mode w/ EGL](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 w/ SSE, Text-mode w/ EGL)
- [LINUX\\_64 Text-mode](#) (Linux (RHEL 6.7 and later) 64-bit Intel/AMD x86\_64 w/ SSE, Text-mode)
- [LINUX MIC-AVX512 Text-mode](#) (Linux (RHEL 6.7 and later) 64-bit Intel Xeon Phi MIC w/ AVX-512, Text-mode, OSPRay)
- [LINUX MIC-AVX512 OpenGL, CUDA, OptiX, OSPRay](#) (Linux (RHEL 6.7 and later) 64-bit Intel Xeon Phi MIC w/ AVX-512, OpenGL, CUDA7.5, OptiX, OSPRay)
- [LINUX OpenPOWER Text-mode](#) (Linux 64-bit IBM OpenPOWER w/ VSX, Text-mode)
- [MacOS X OpenGL \(32-bit Intel x86\)](#) (Apple MacOS-X (10.4.7 to 10.13.x) with hardware OpenGL (native bundle))
- [Windows OpenGL, CUDA \(Windows XP/Vista/7/8/10 \(32-bit\) with OpenGL and CUDA\)](#)
- [Windows OpenGL \(32-bit Intel x86\)](#) (Microsoft Windows XP/Vista/7/8/10 (32-bit) using OpenGL)
- [NCSA Blue Waters \(Cray XK7 w/ OpenGL\)](#) (NCSA Blue Waters (Cray XK7) MPI, CUDA, OpenGL Pbuffers, TachyonL-OptiX)
- [ORNL Titan \(Cray XK7\)](#) (ORNL Titan (Cray XK7) MPI, CUDA, TachyonL-OptiX)
- [CSCS Piz Daint \(Cray XC50 w/ EGL\)](#) (CSCS Piz Daint (Cray XC50) MPI, CUDA, EGL Pbuffers, TachyonL-OptiX)

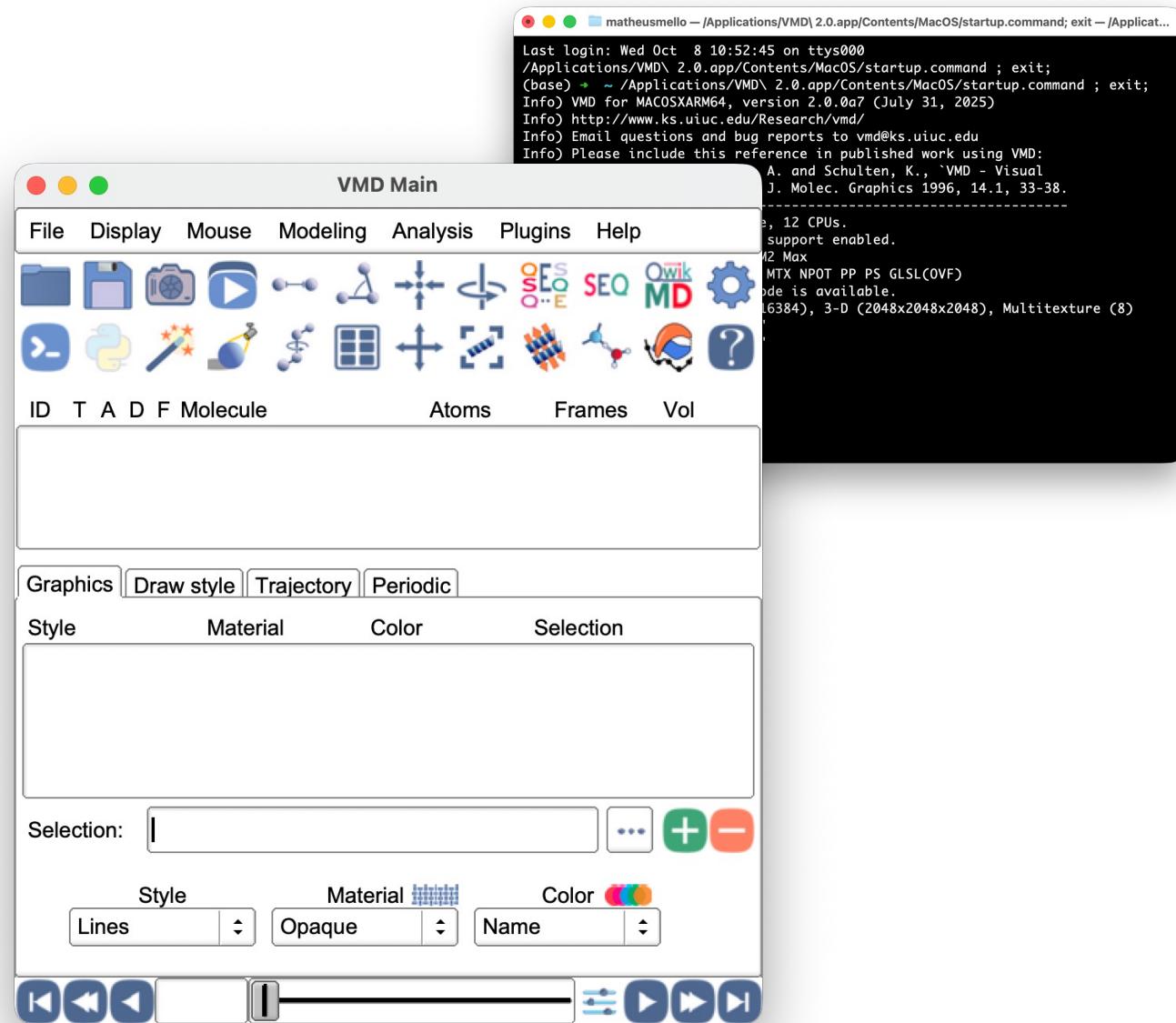
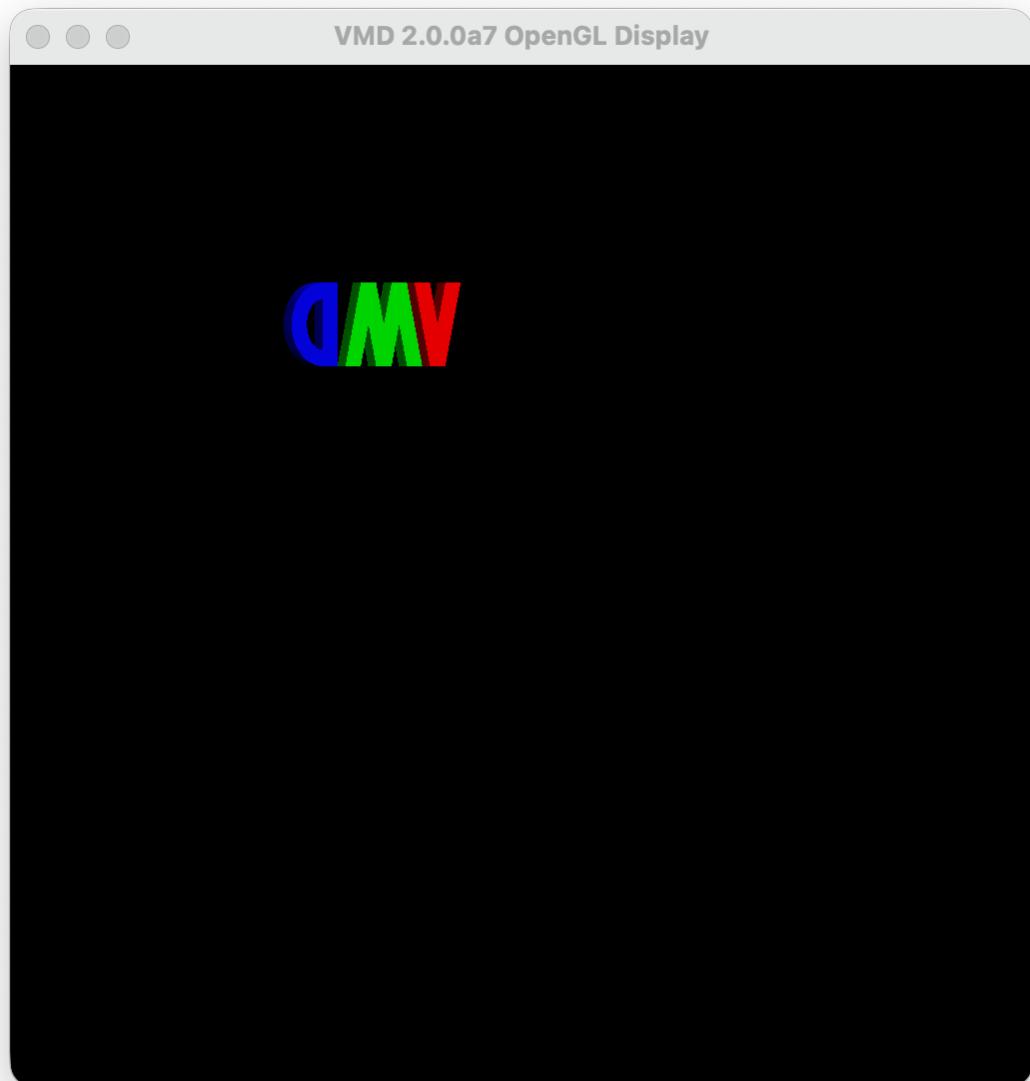
**Version 1.9.2 (2014-12-29) Platforms:**

We recommend that all users upgrade to VMD 1.9.3

- [Source Code](#)
- [LINUX\\_64 OpenGL, CUDA, Text-based OptiX](#) (Linux (RHEL 5 and later) 64-bit Intel/AMD x86\_64 SSE, with CUDA and Text-based OptiX)

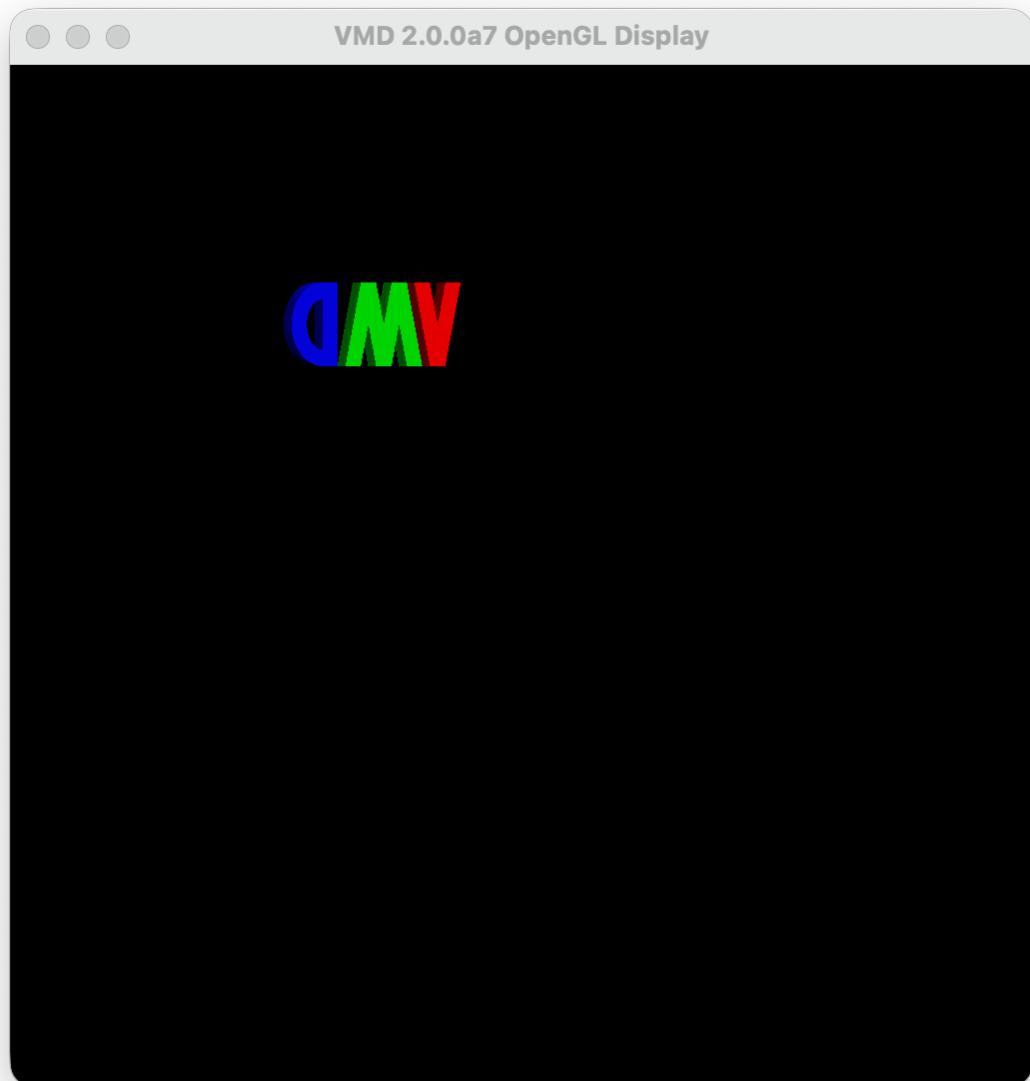
Select  
platform

# Opening VMD

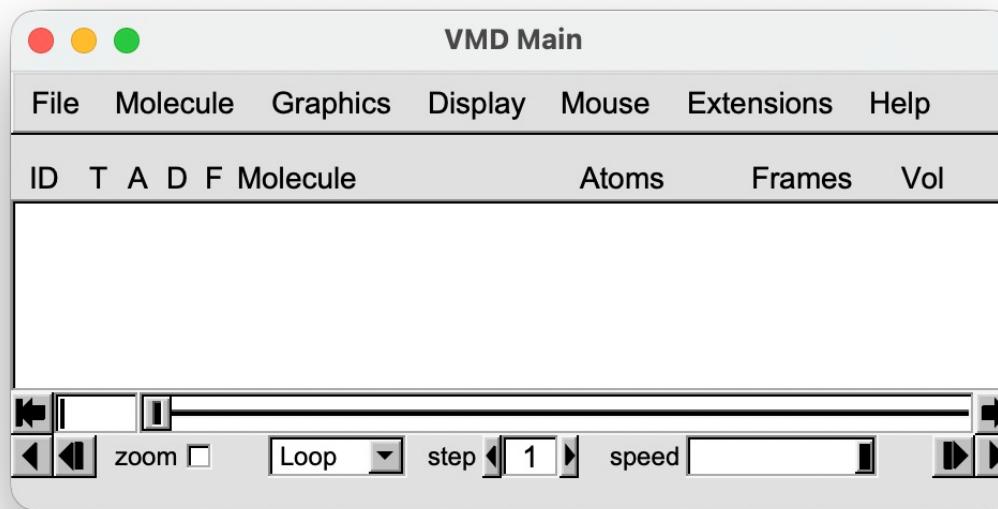


version 2.0.0

# Opening VMD

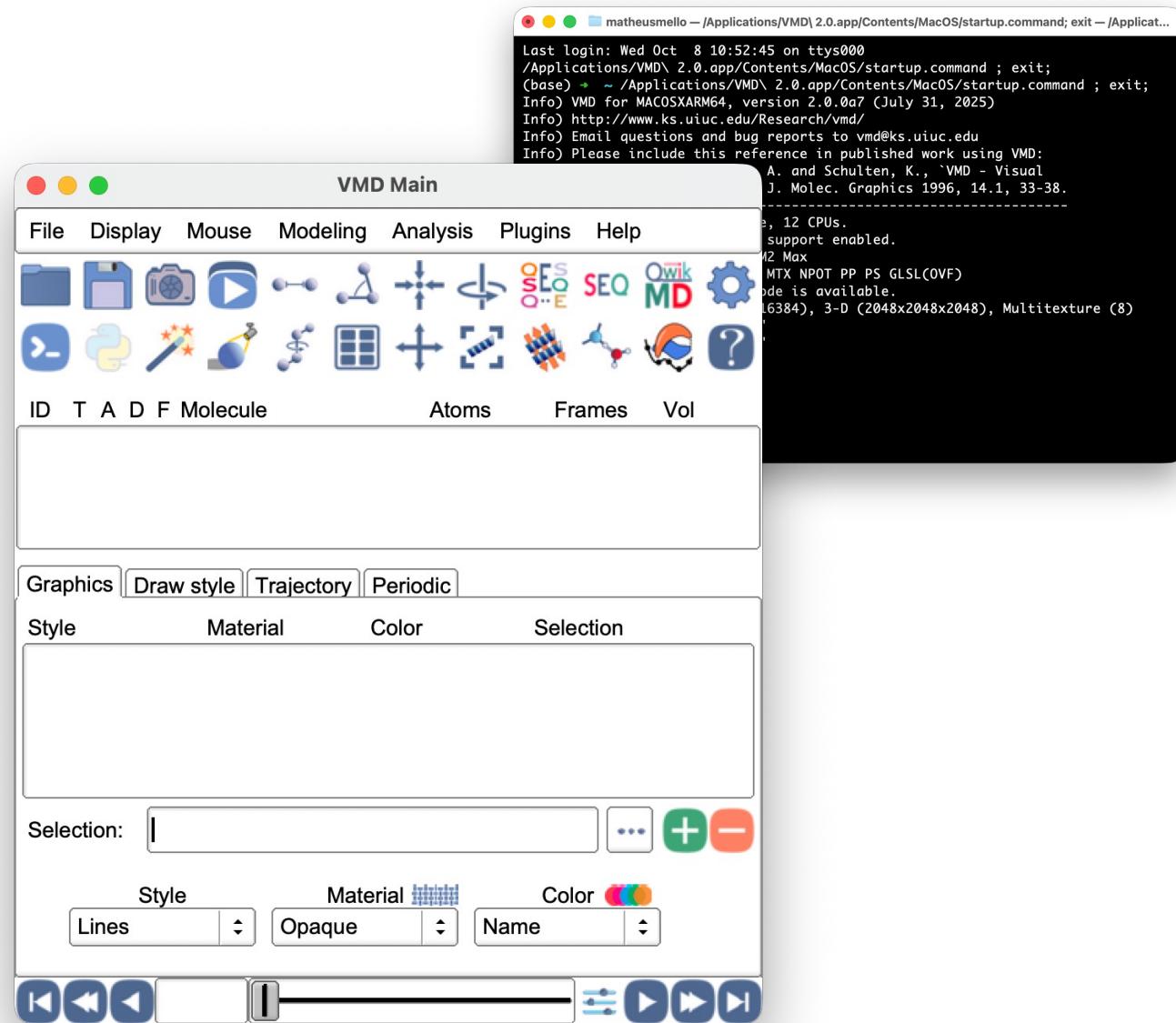
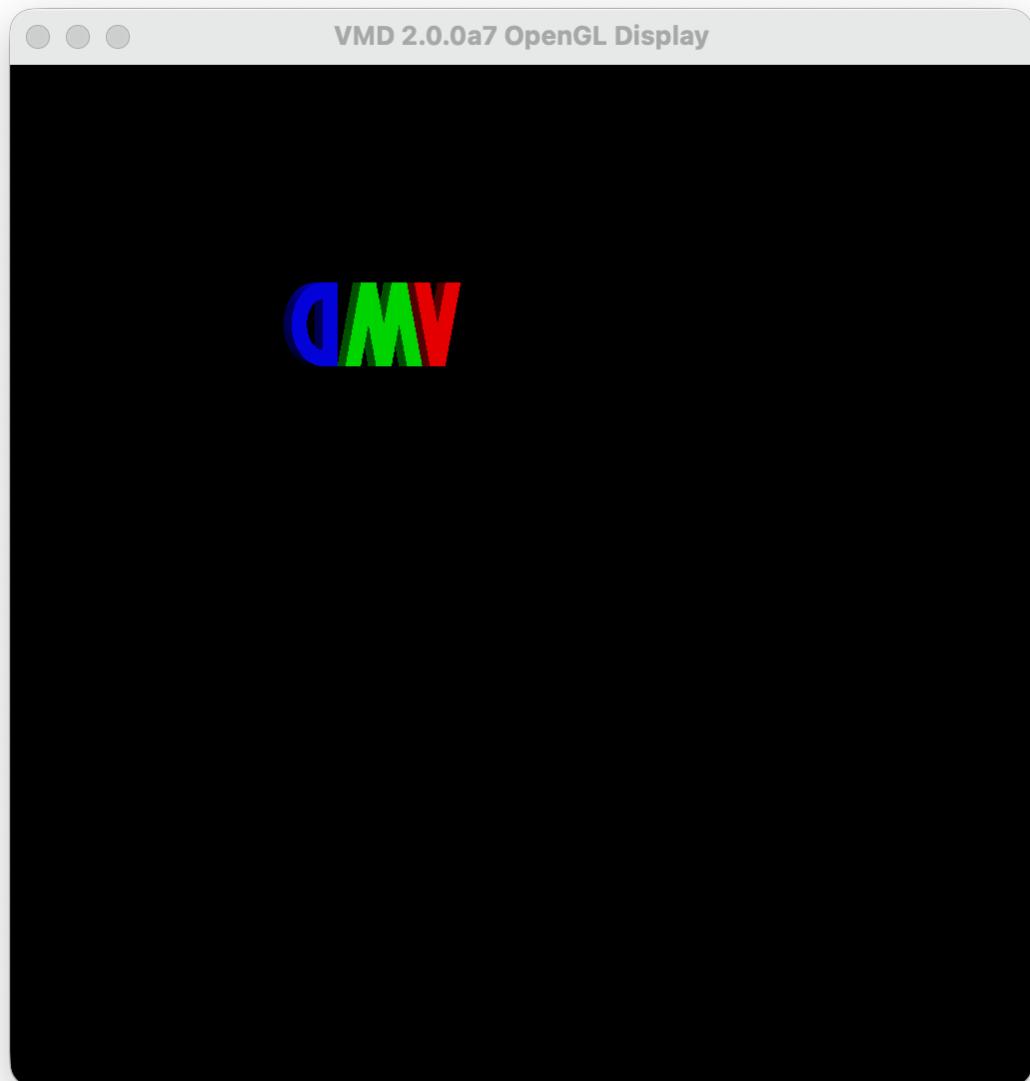


```
matheusmello — /Applications/VMD\ 2.0.app/Contents/MacOS/startup.command; exit — /Appli...
Last login: Wed Oct  8 10:52:45 on ttys000
/Applications/VMD\ 2.0.app/Contents/MacOS/startup.command ; exit;
(base) ~ /Applications/VMD\ 2.0.app/Contents/MacOS/startup.command ; exit;
Info) VMD for MACOSXARM64, version 2.0.0a7 (July 31, 2025)
Info) http://www.ks.uiuc.edu/Research/vmd/
Info) Email questions and bug reports to vmd@ks.uiuc.edu
Info) Please include this reference in published work using VMD:
Info)   Humphrey, W., Dalke, A. and Schulten, K., 'VMD - Visual
Info)   Molecular Dynamics', J. Molec. Graphics 1996, 14.1, 33-38.
Info) -----
Info) Multithreading available, 12 CPUs.
Info) High-DPI OpenGL display support enabled.
Info) OpenGL renderer: Apple M2 Max
Info)   Features: STENCIL MDE MTX NPOT PP PS GLSL(OVF)
Info)   Full GLSL rendering mode is available.
Info)   Textures: 2-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
ERROR) Duplicate resname "4YS"
ERROR) Duplicate resname "YGA"
after#0
vmd >
```



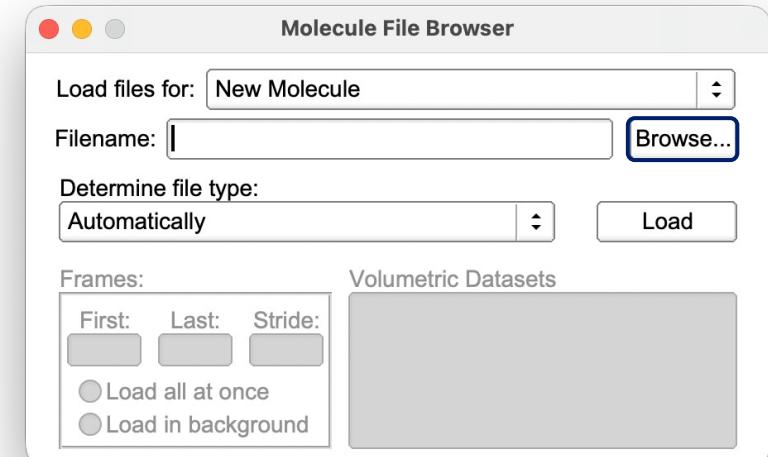
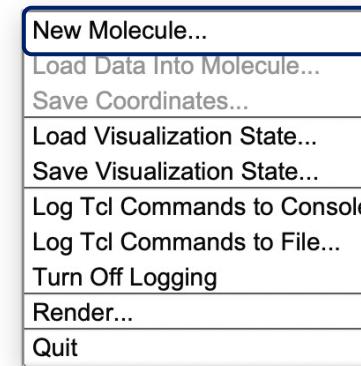
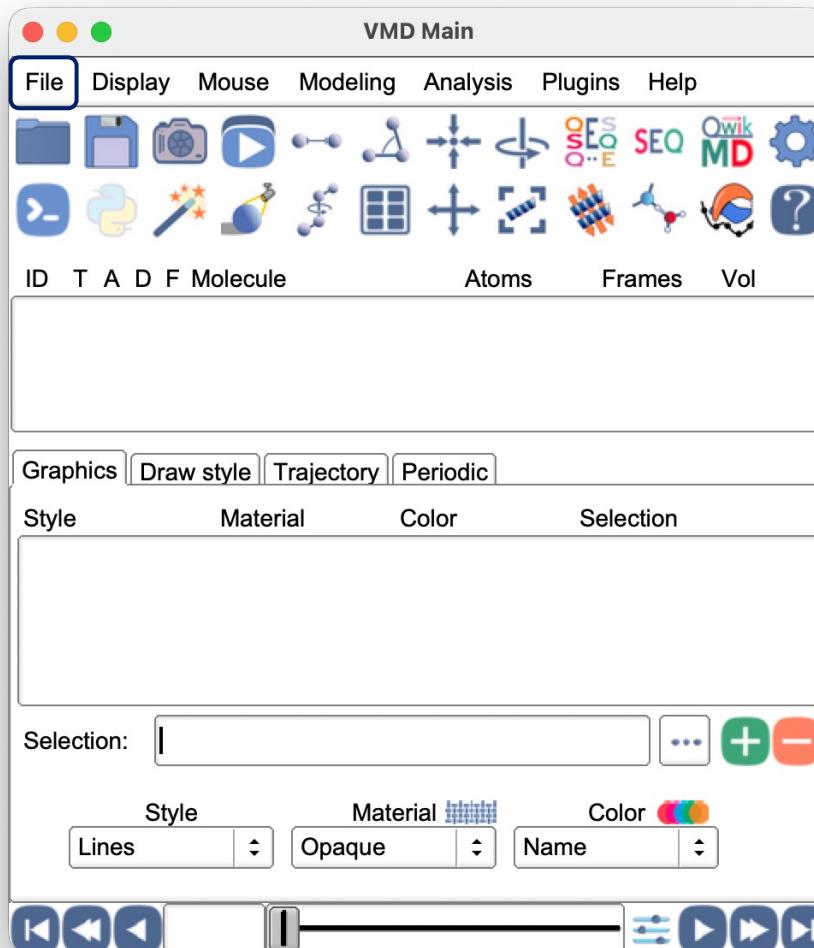
version 1.9.4

# Opening VMD



version 2.0.0

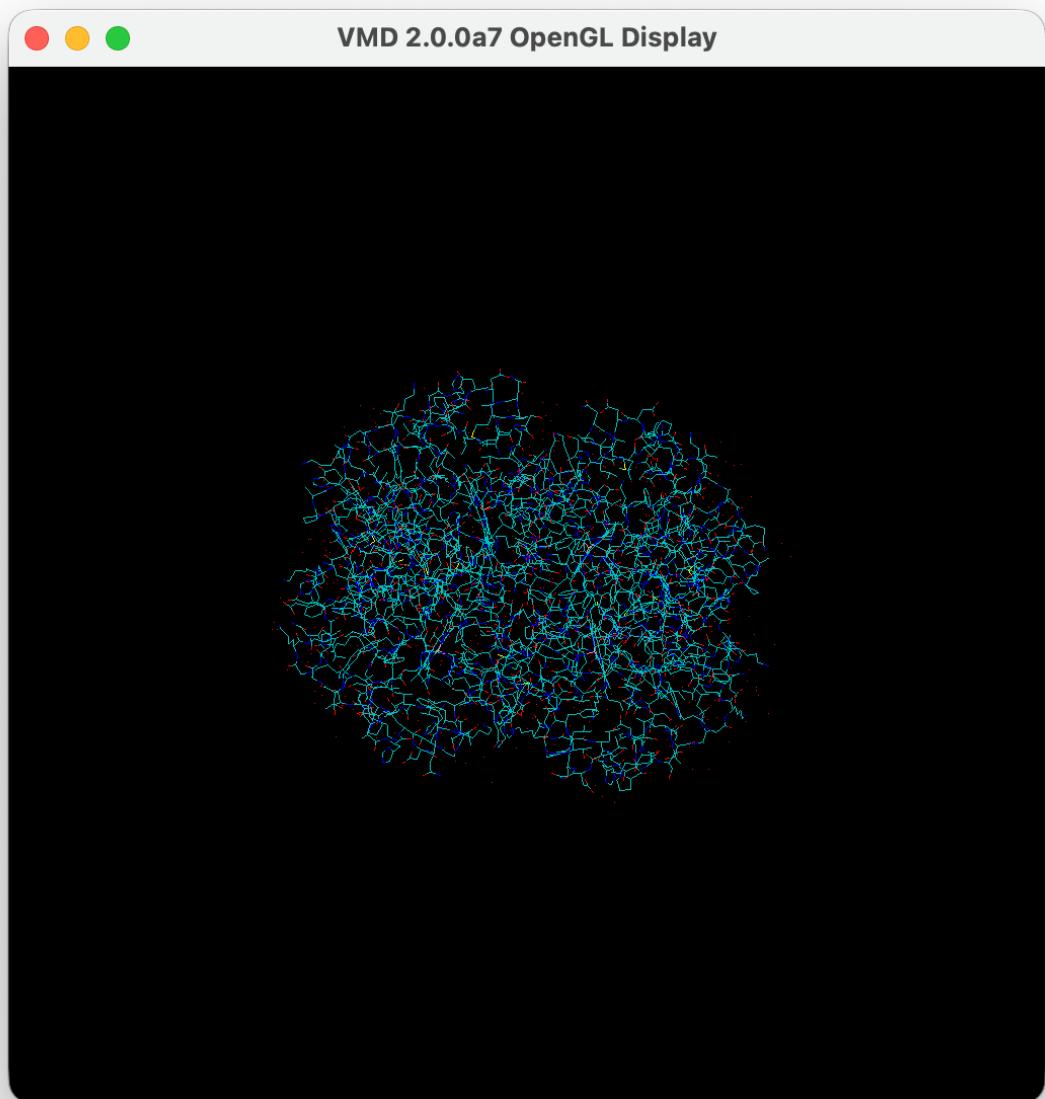
# Loading a molecule



Download PDB

Also at: <https://github.com/Whitford/ctbp-techtalks>

# Loading a molecule



VMD Main

File Display Mouse Modeling Analysis Plugins Help

OS OEE SEQ Qwik MD

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	1A3N.pdb	4997	1	0

Graphics Draw style Trajectory Periodic

Style	Material	Color	Selection
Lines	Opaque	Name	all

Selection: all

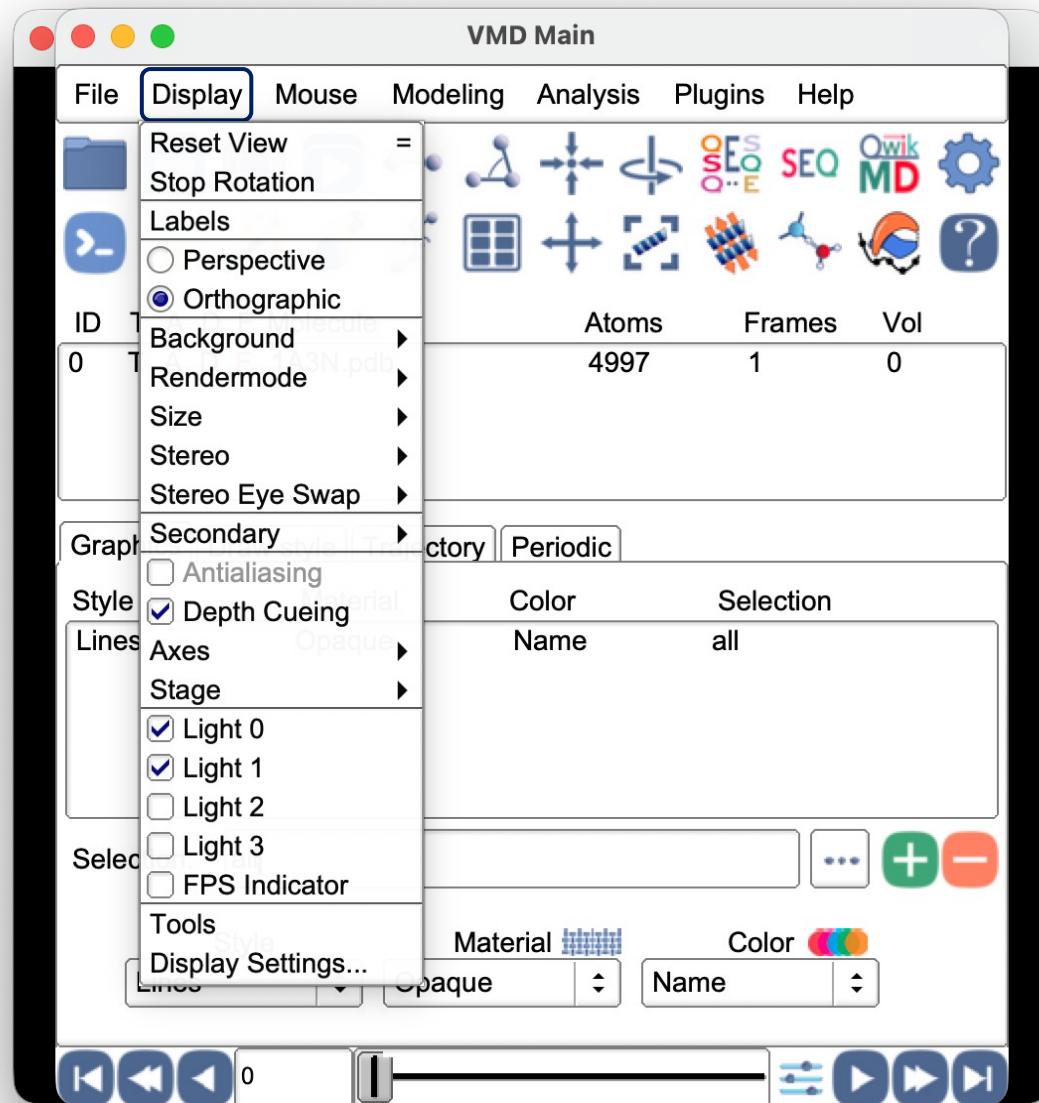
Style Material Color

Lines	Opaque	Name
-------	--------	------

0

version 2.0.0

# Changing Display options



We can change under **Display**:

Perspective > Orthographic

Axes > Off

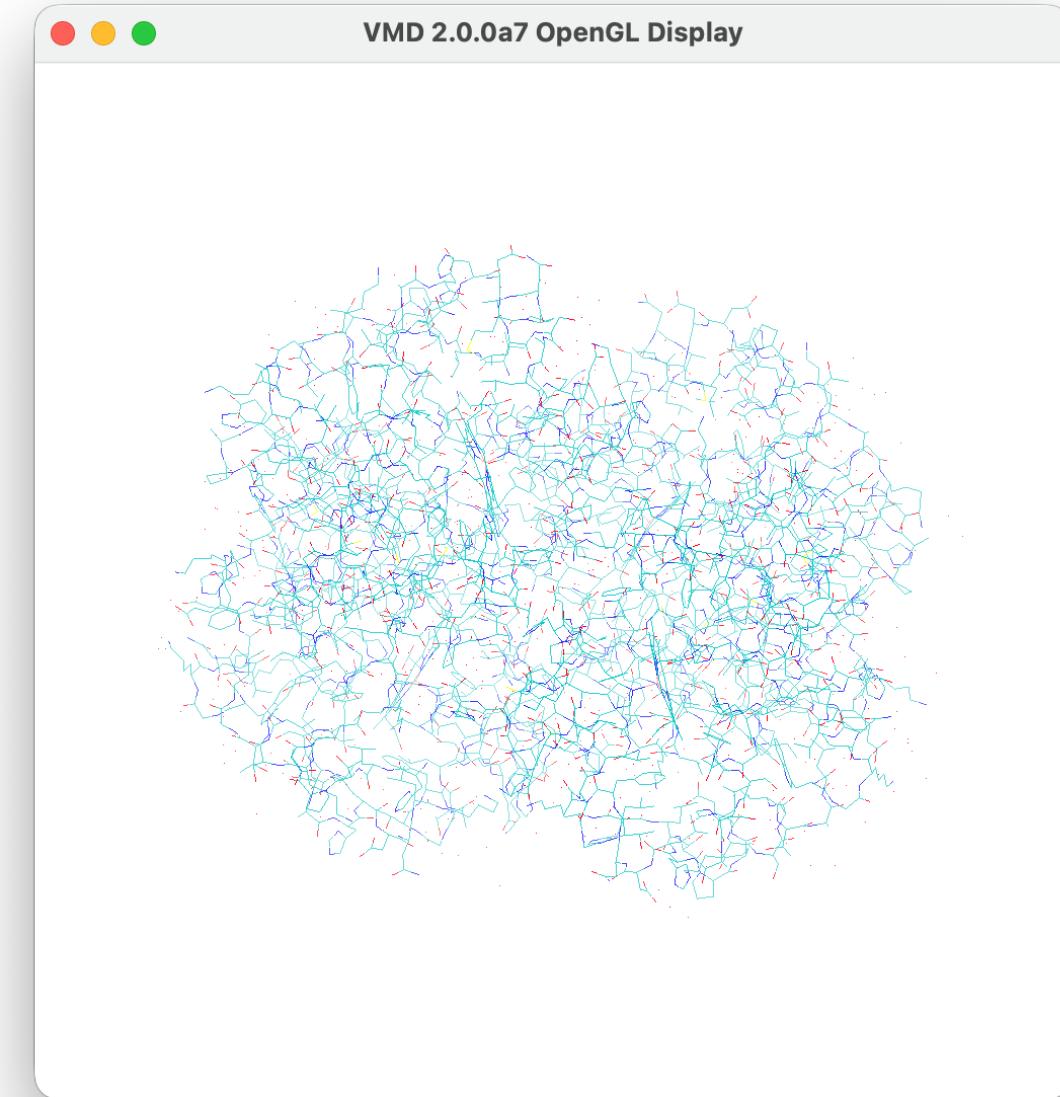
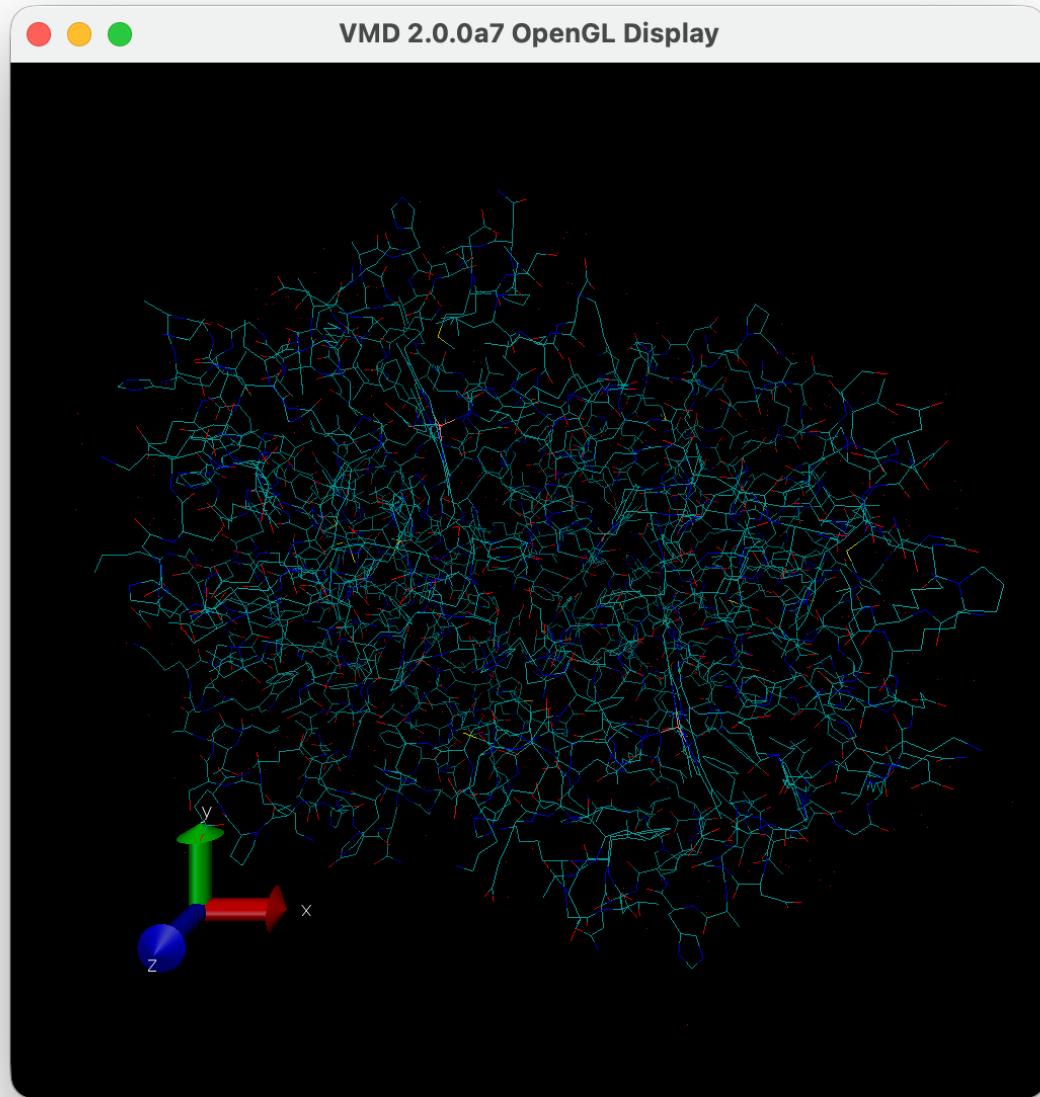
Background > White



In version 1.9.4

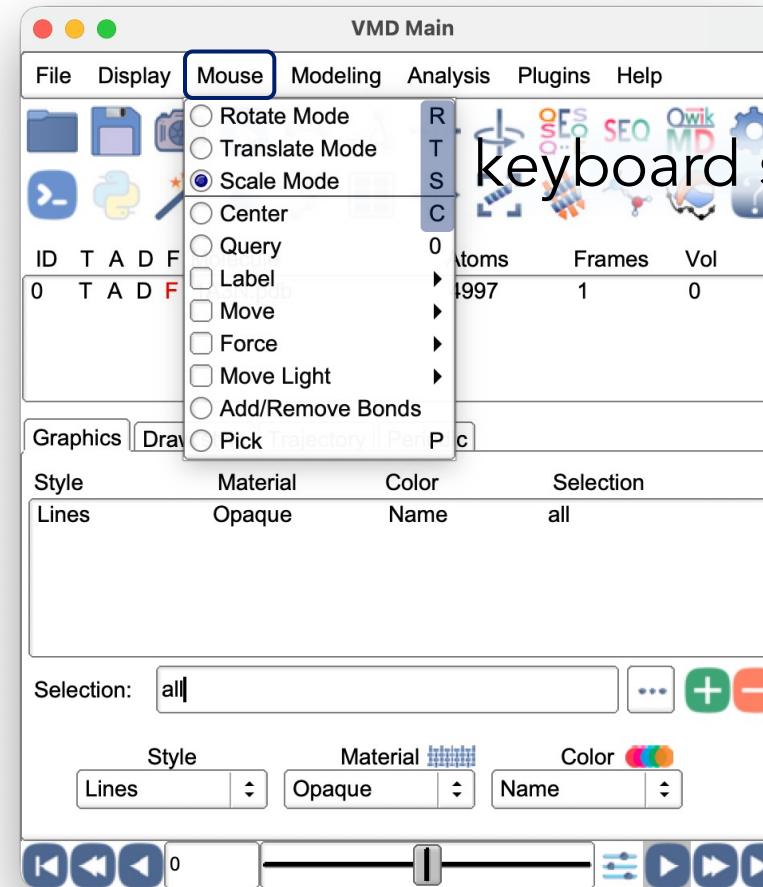
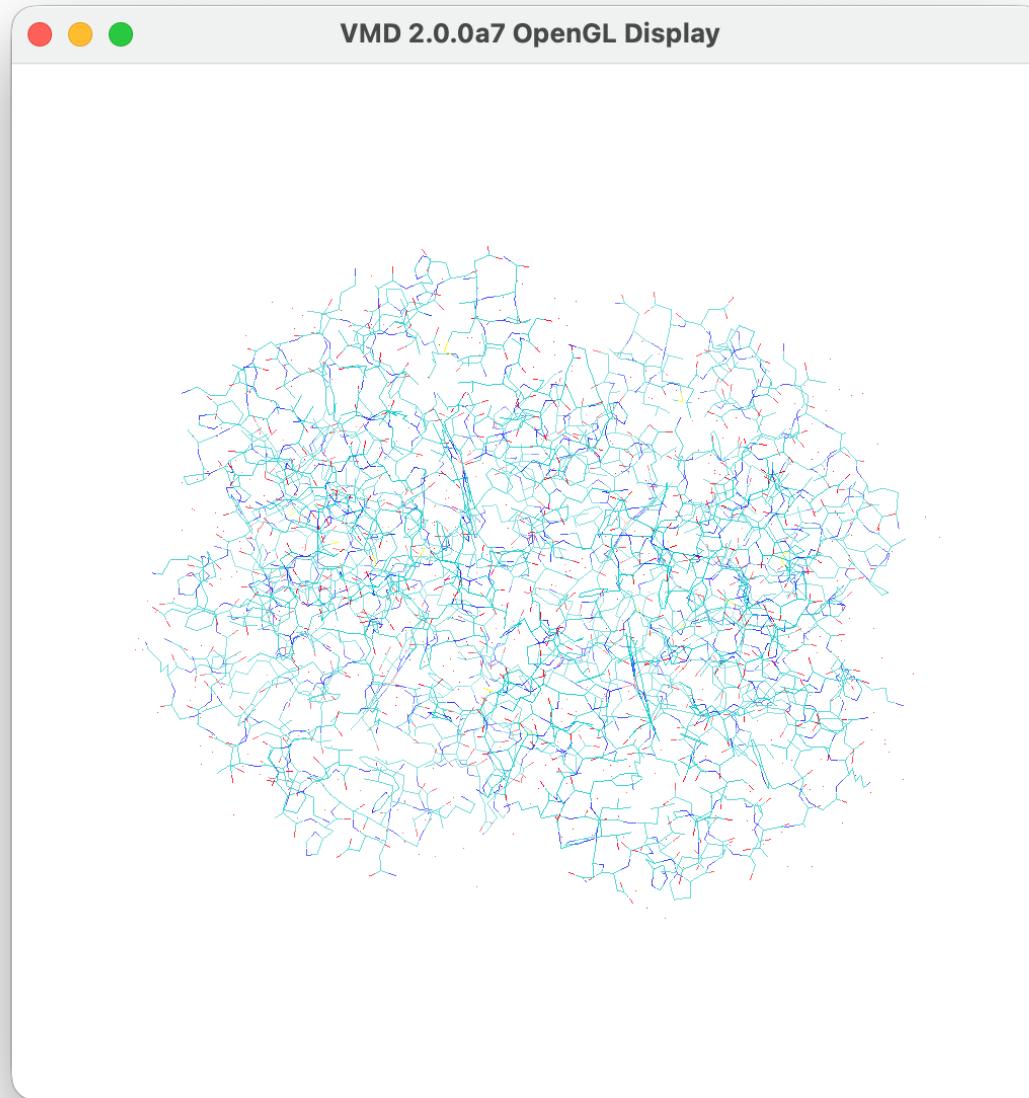
Graphics > Colors > Display > Background

# Changing Display options



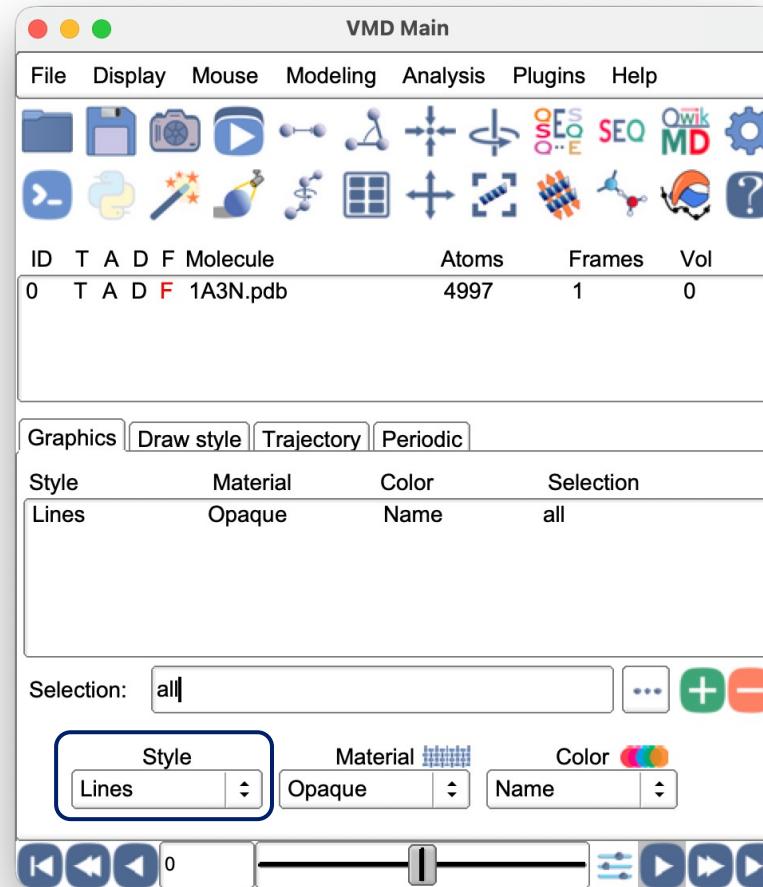
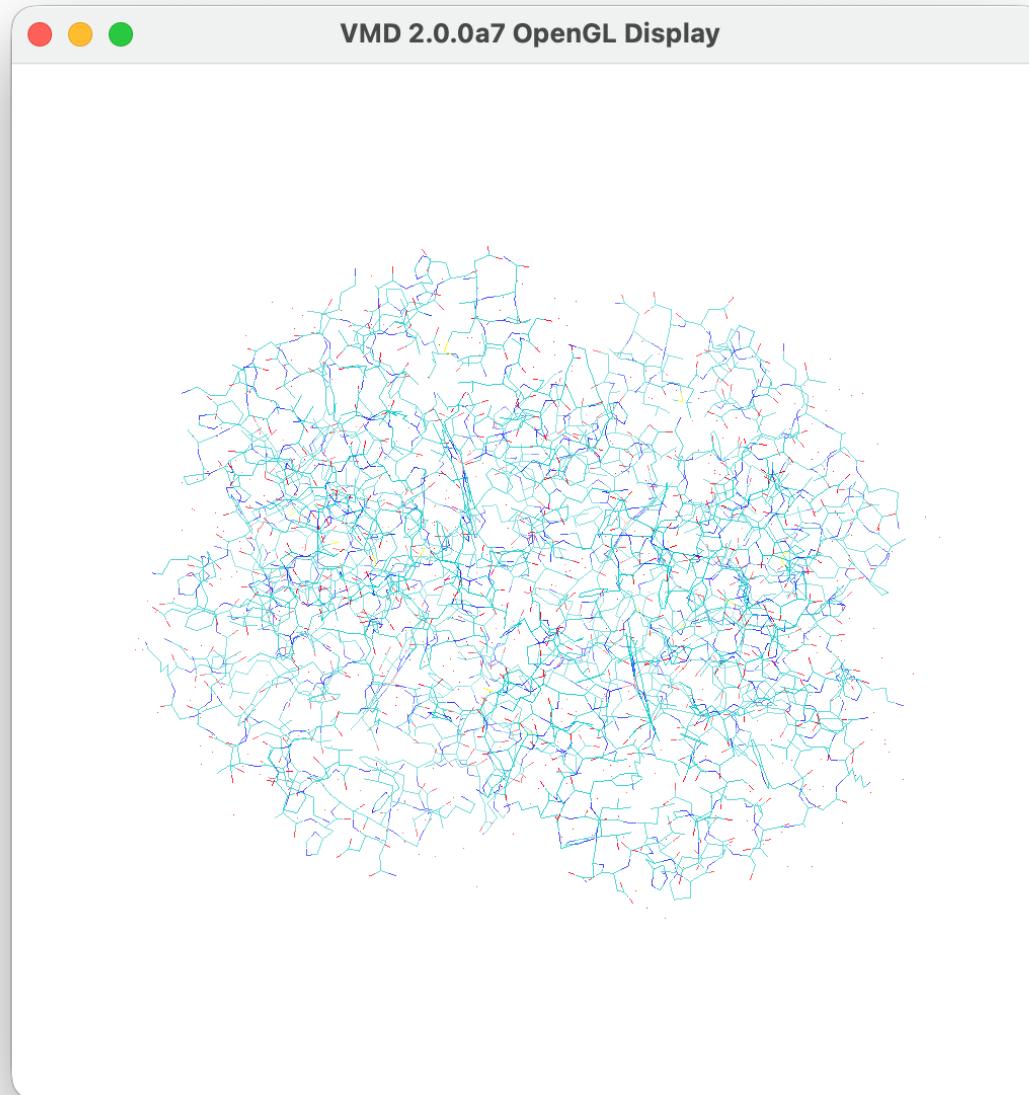
version 2.0.0

# Exploring mouse actions



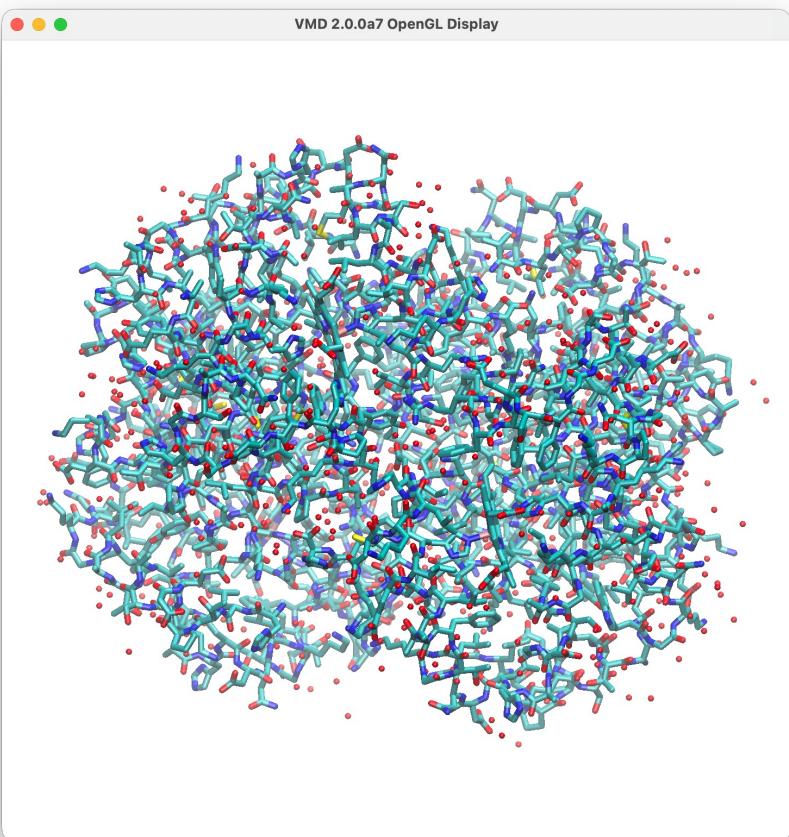
keyboard shortcuts

# Changing the representation style

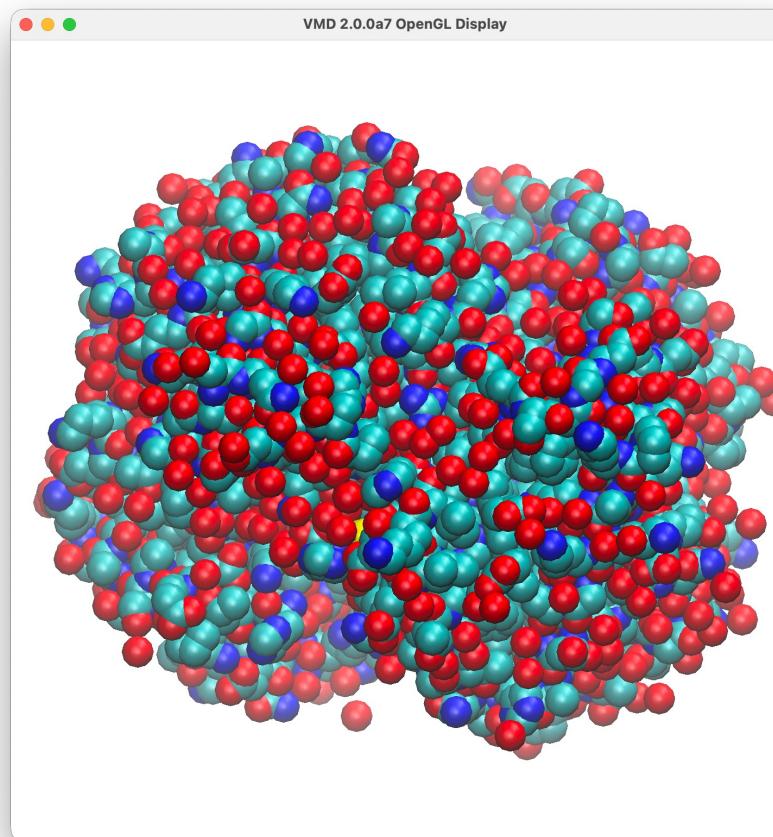


# Changing the representation style

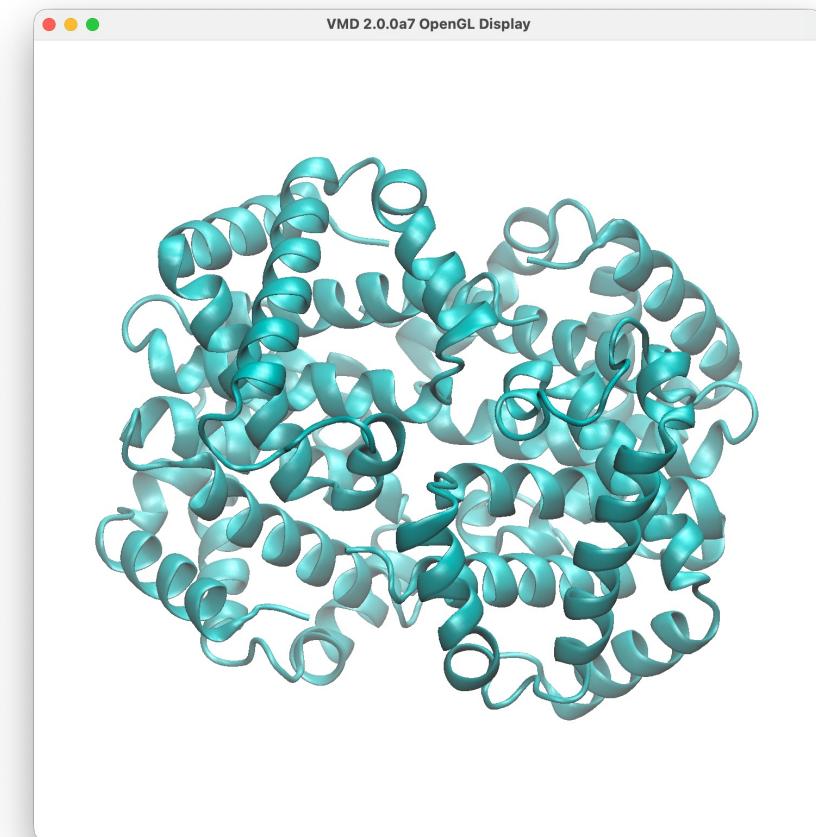
Licorice



VDW



NewCartoon

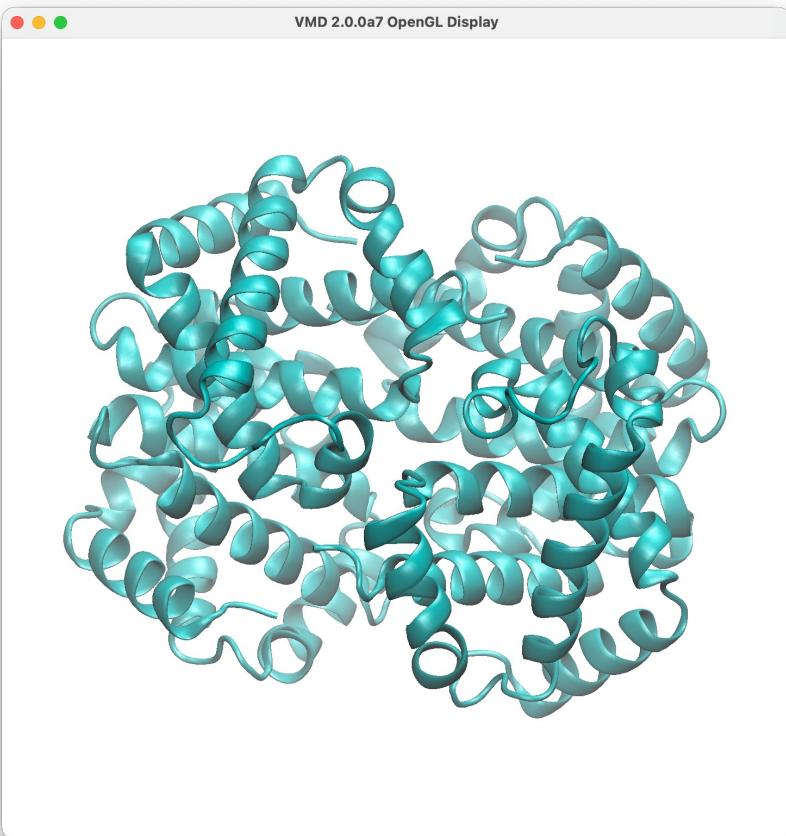


Style  Material  Color

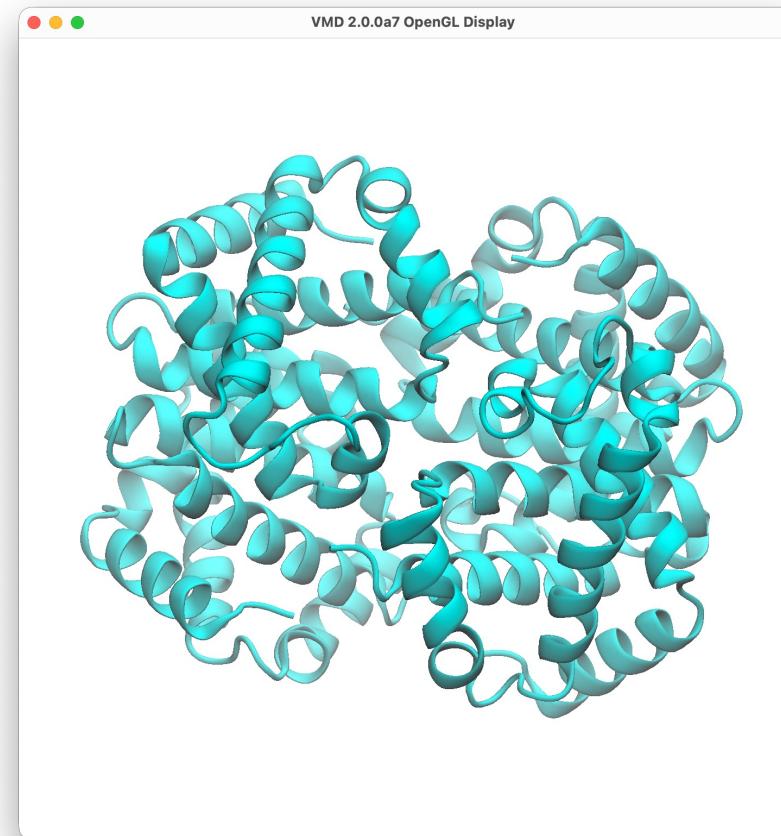
version 2.0.0

# Changing the representation material

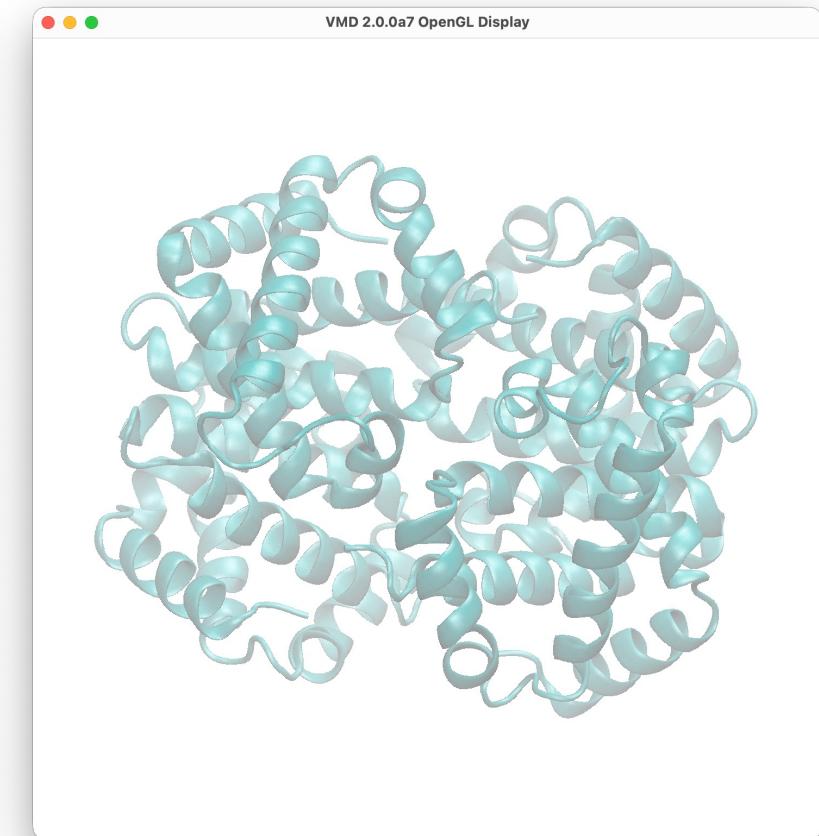
Opaque



A0Chalky



Transparent



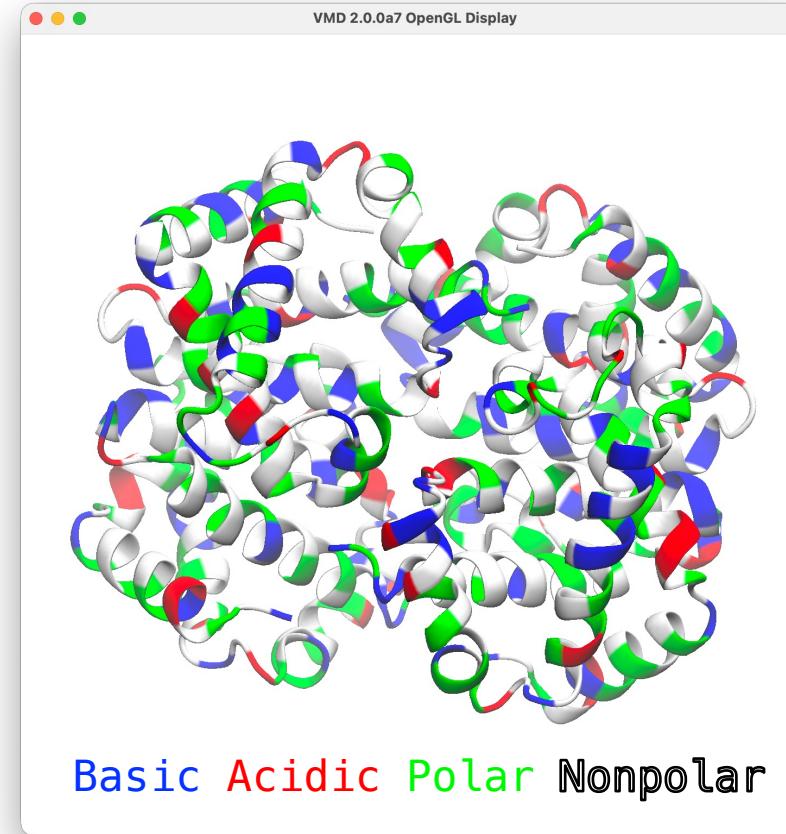
version 2.0.0

# Changing the representation colors

ColorID (31)



ResType



Chain

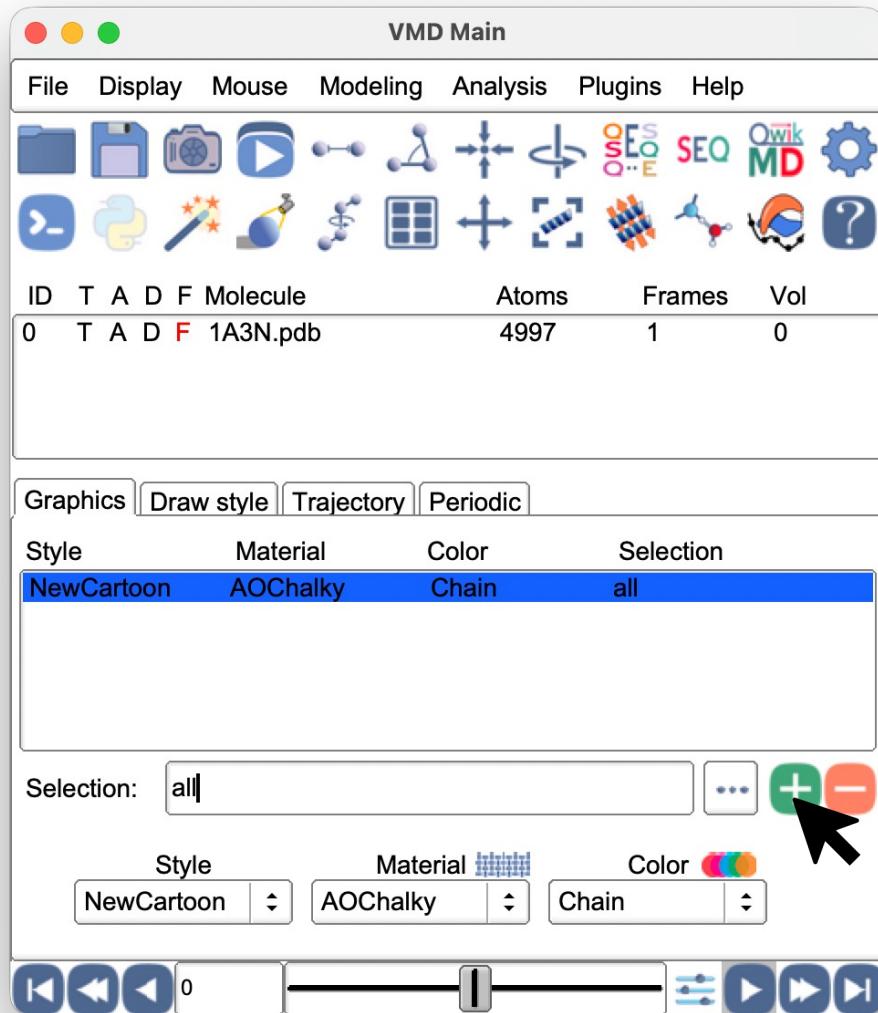


Basic Acidic Polar Nonpolar

Style  Material  Color  Name

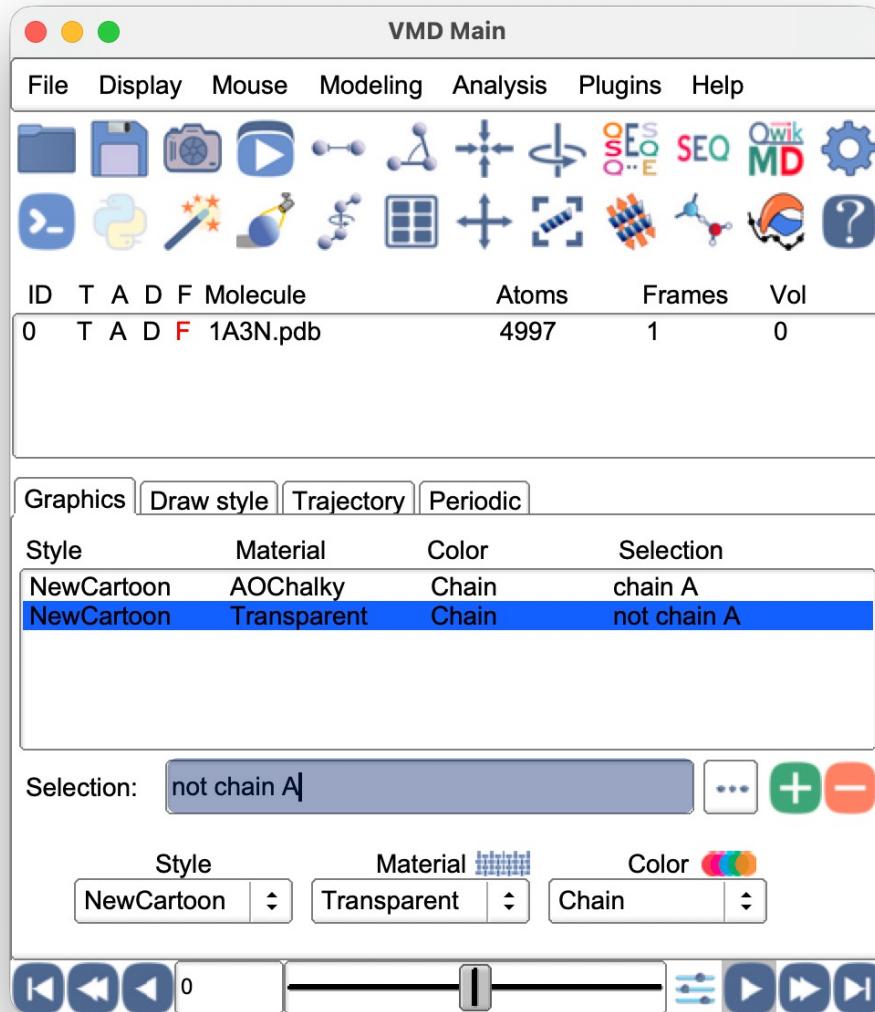
version 2.0.0

# Adding different representations and selections

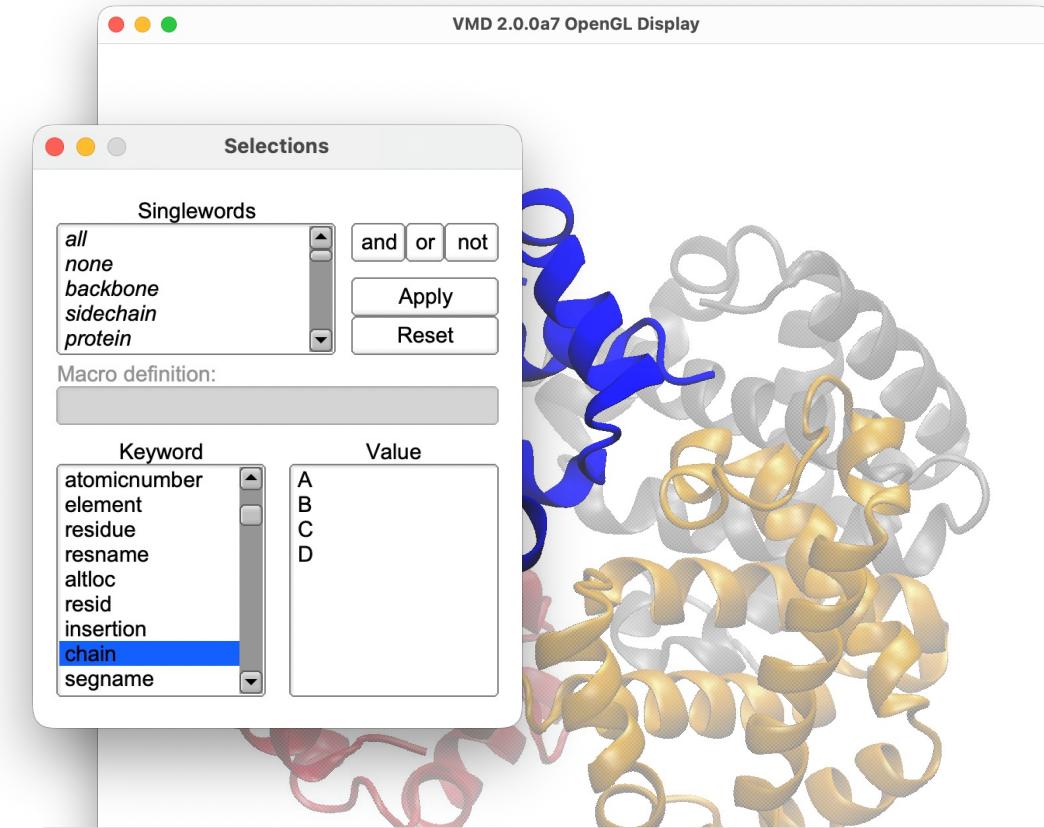
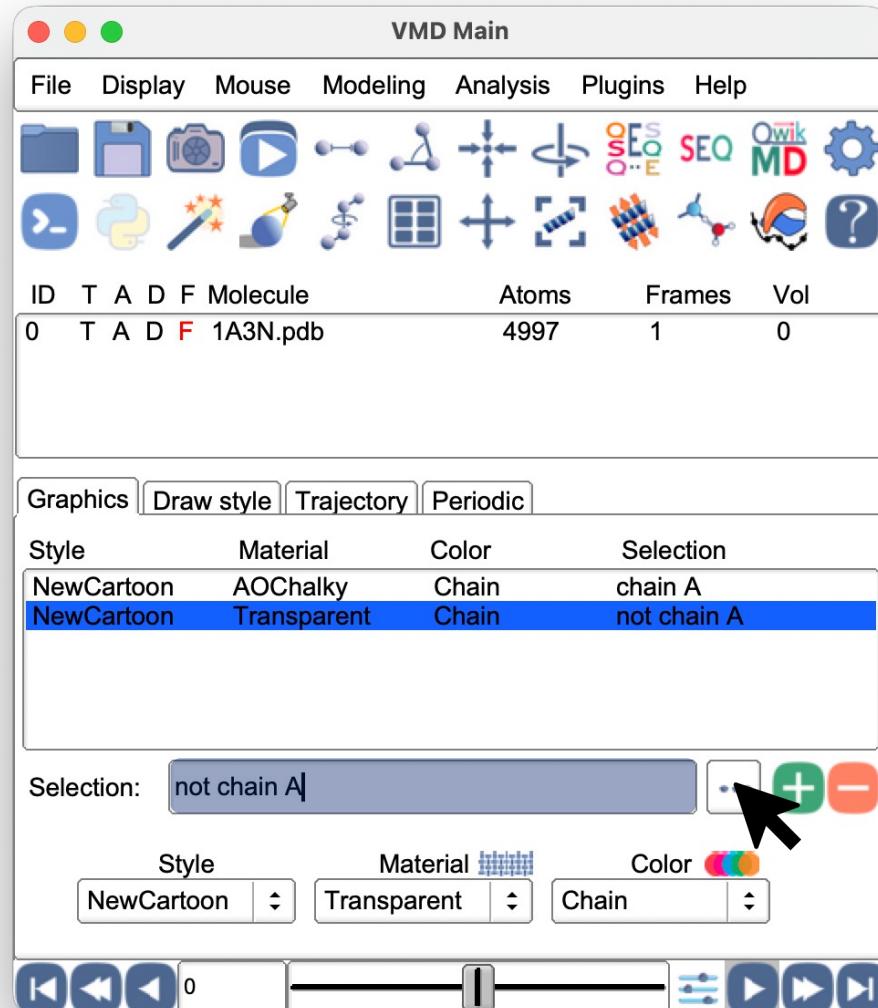


version 2.0.0

# Adding different representations and selections

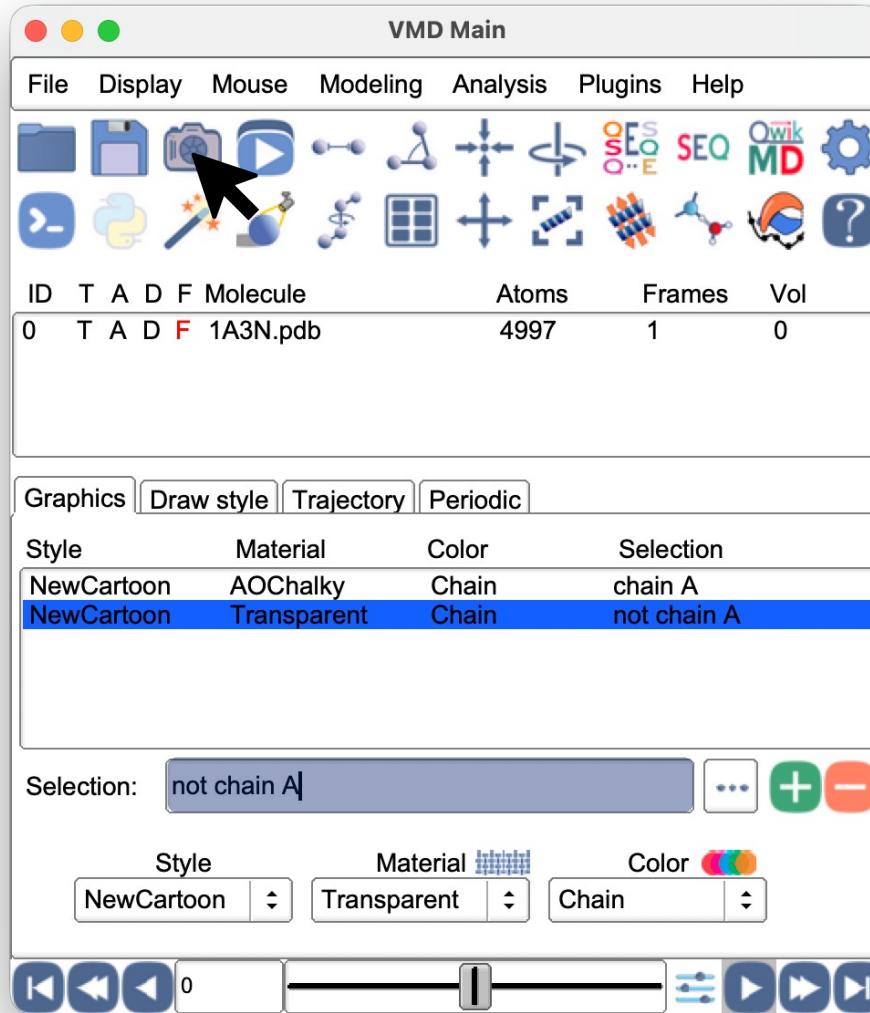


# Adding different representations and selections

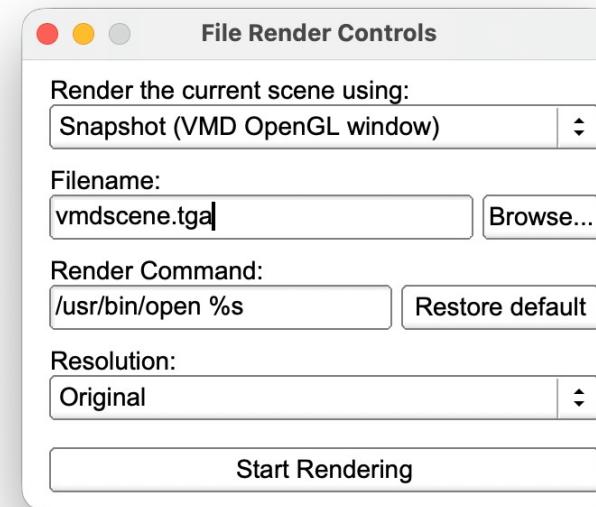


Selections window helps identify possible selections

# Rendering images



Alternatively: File > Render  
(version 1.9.4)



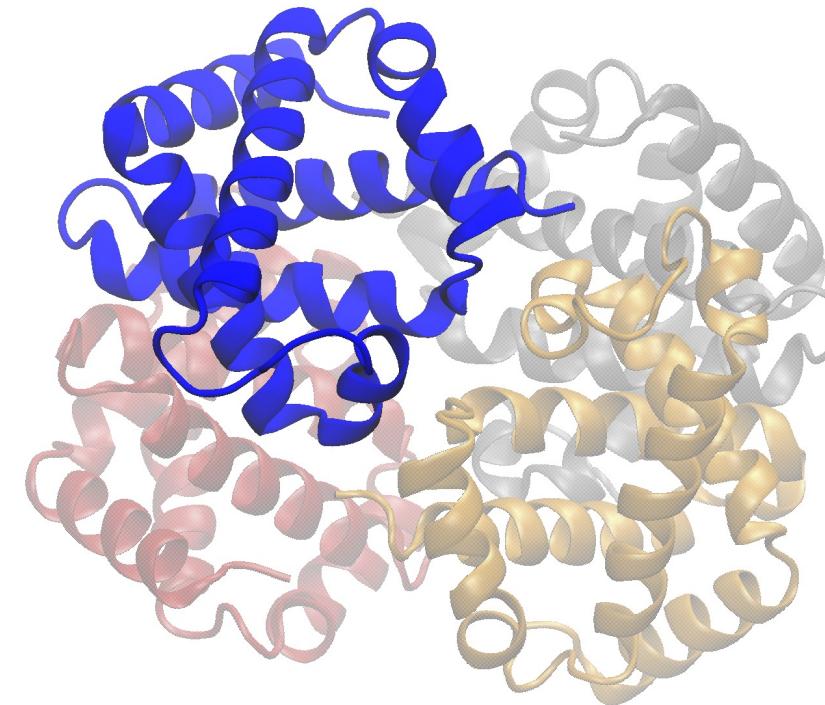
rendering engine  
folder/file name

version 2.0.0

# Rendering images



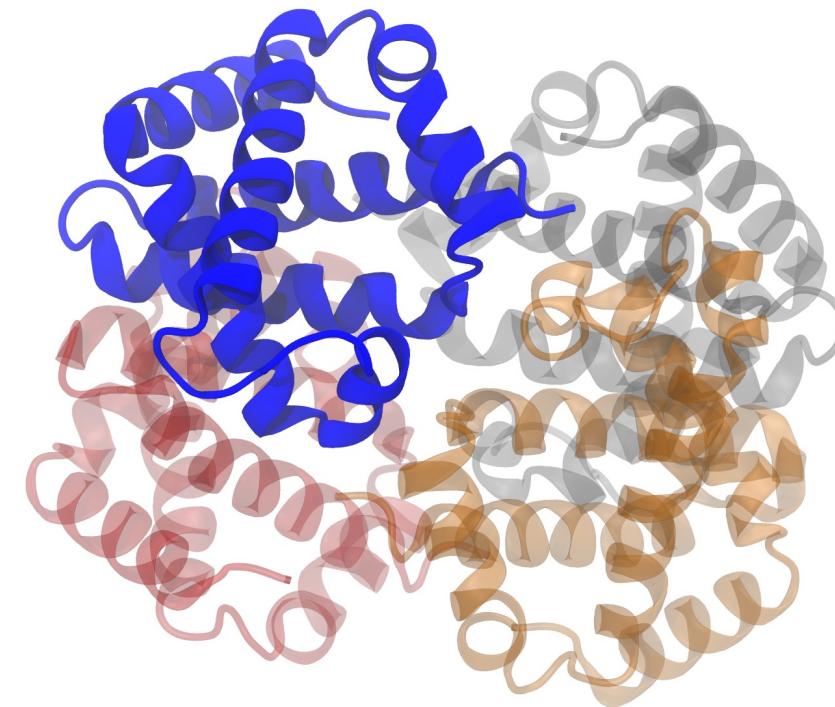
Snapshot



# Rendering images

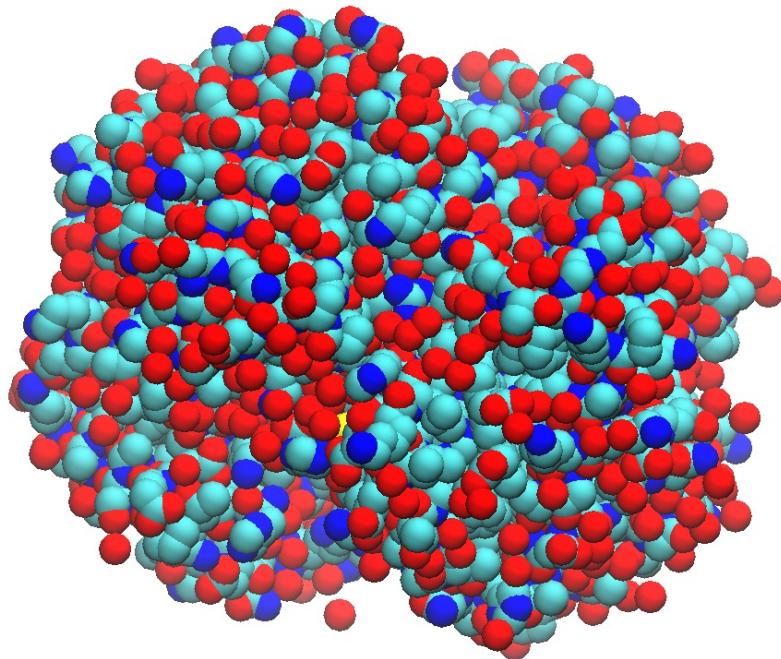


Tachyon Internal

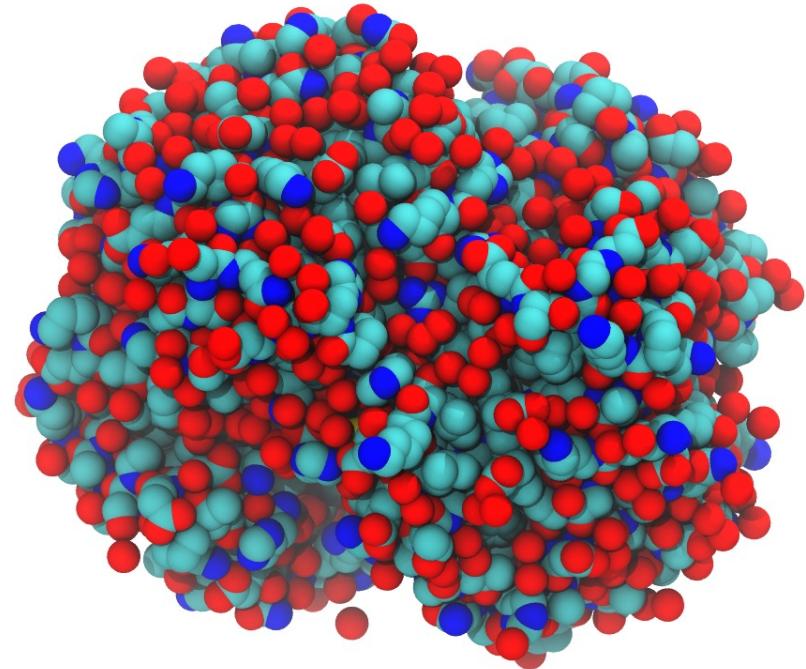


# Rendering images

Snapshot



Tachyon Internal

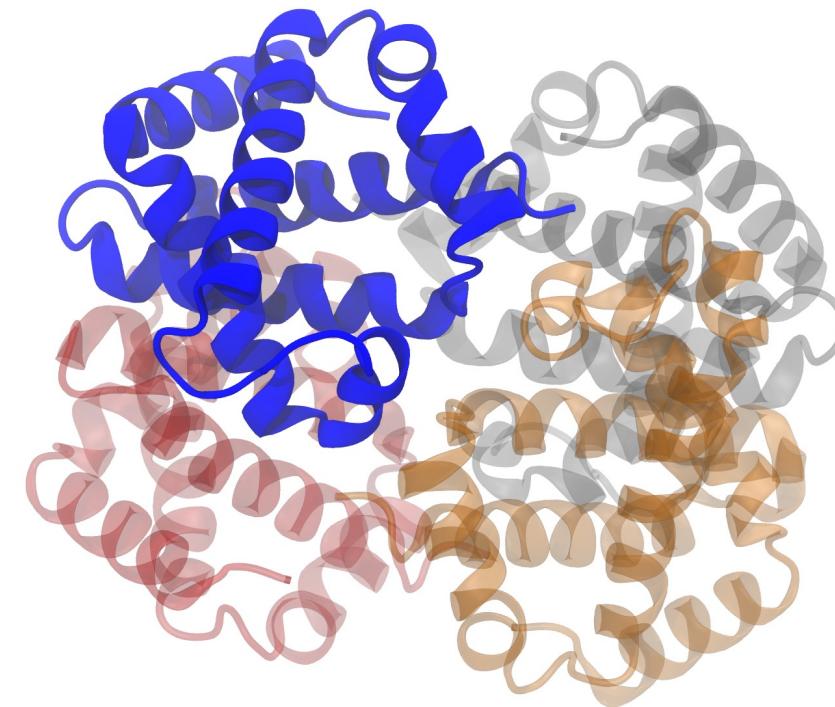


Shadows and the depth cueing  
become more apparent in Tachyon

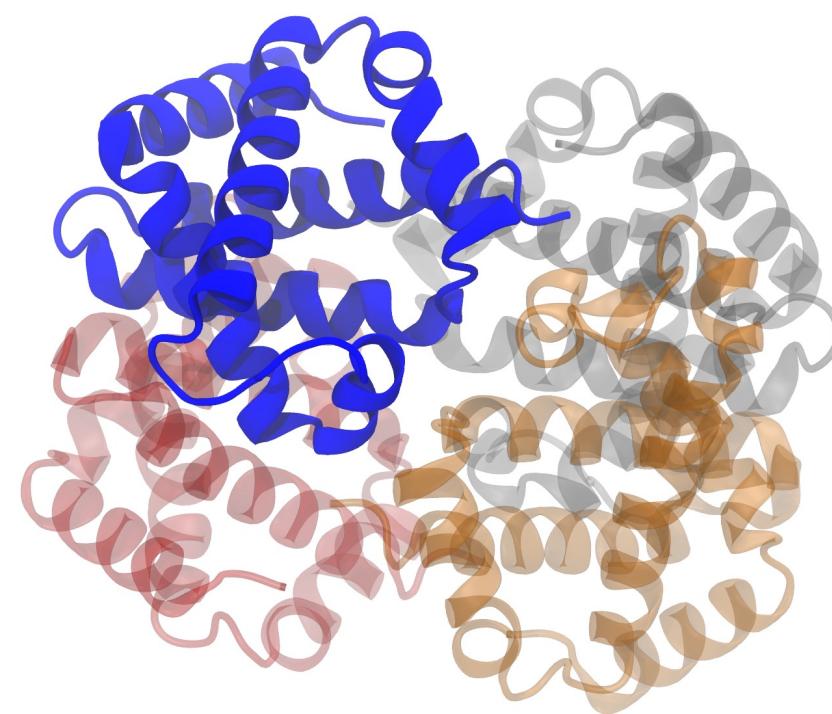
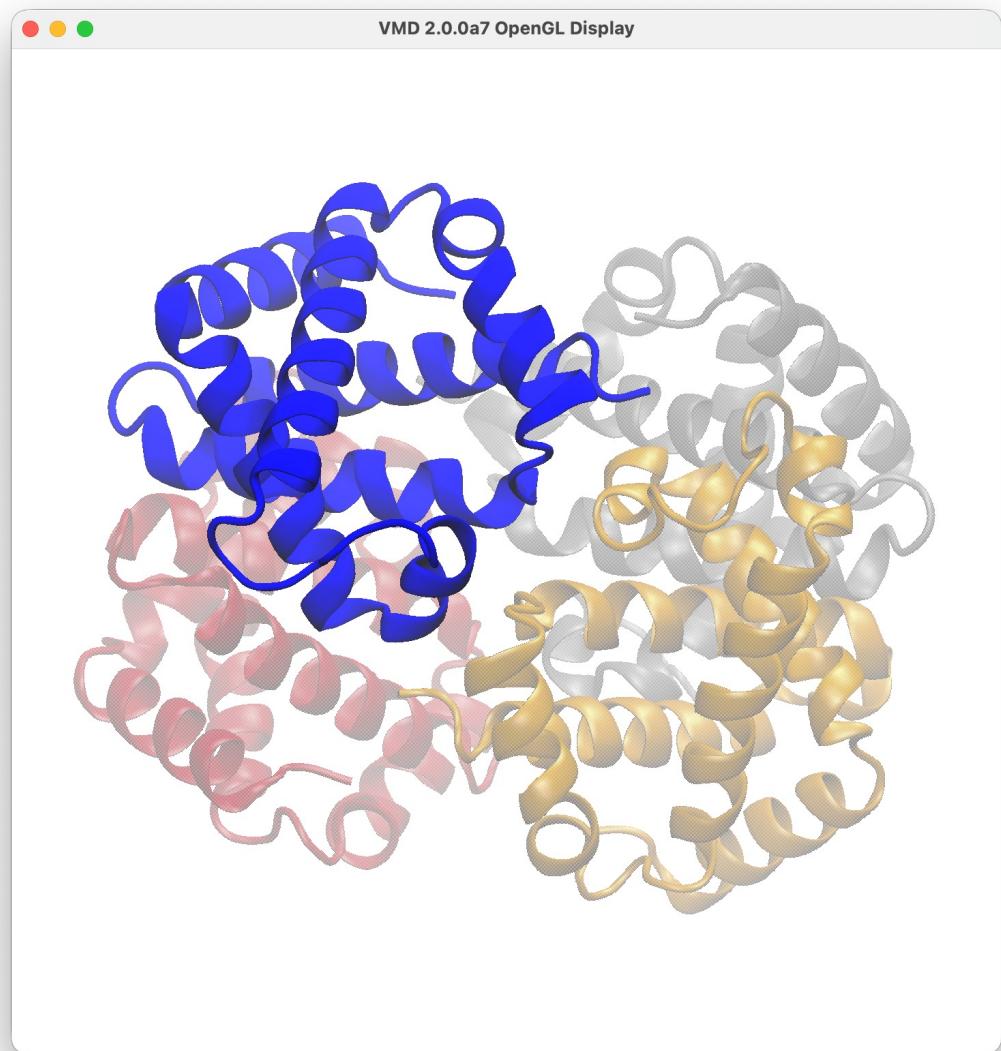
# Rendering images



Tachyon Internal

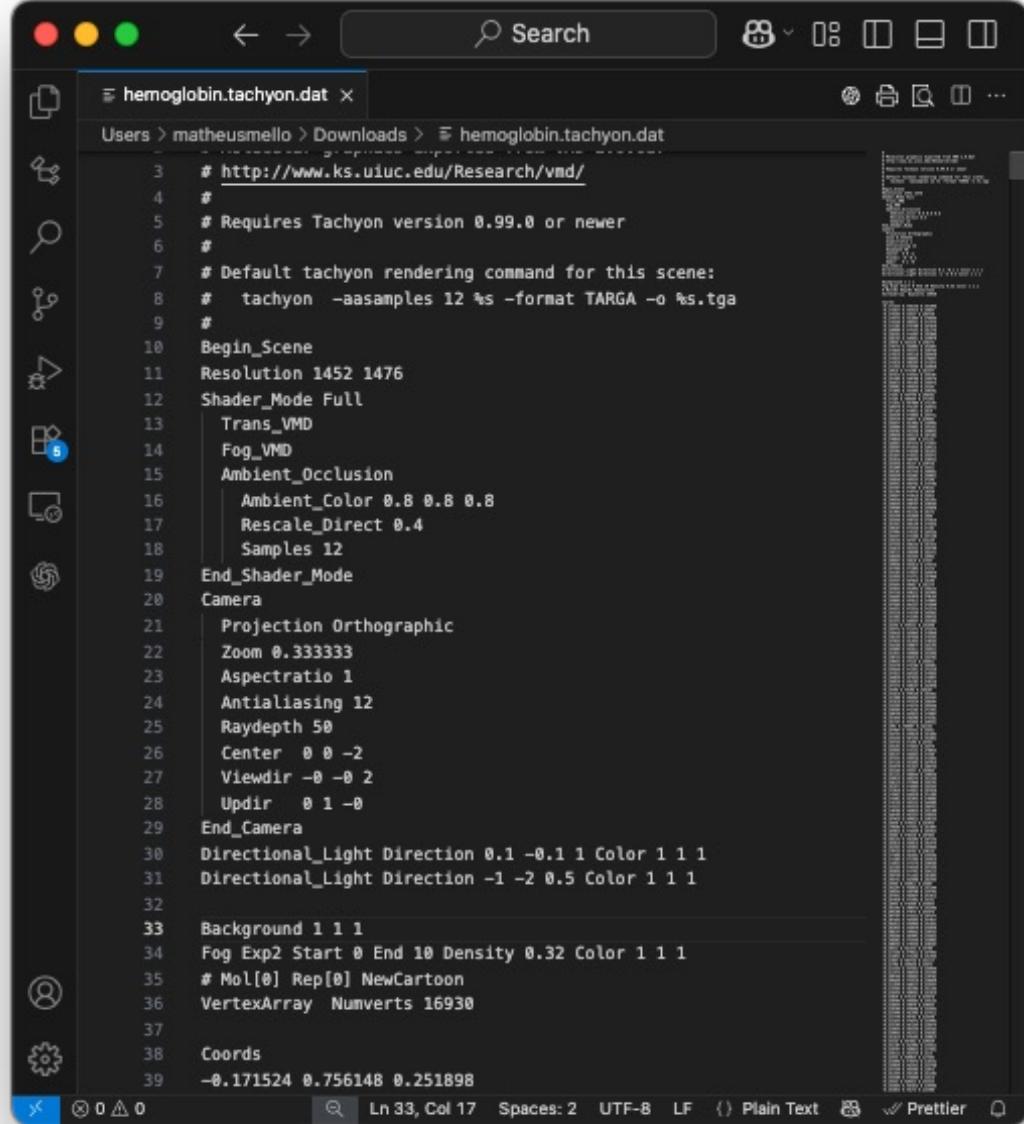


# Rendering images



Note that a .dat file was generated

# Rendering images



A screenshot of a Mac OS X terminal window titled "hemoglobin.tachyon.dat". The window shows a text-based configuration file for a rendering scene. The file includes directives for rendering command, resolution, shader mode, ambient occlusion, camera projection, and various lighting parameters. The terminal interface has a dark theme with light-colored text.

```
hemoglobin.tachyon.dat
Users > matheusmello > Downloads > hemoglobin.tachyon.dat
3 # http://www.ks.uiuc.edu/Research/vmd/
4 #
5 # Requires Tachyon version 0.99.0 or newer
6 #
7 # Default tachyon rendering command for this scene:
8 # tachyon -aasamples 12 %s -format TARGA -o %s.tga
9 #
10 Begin_Scene
11 Resolution 1452 1476
12 Shader_Mode Full
13 Trans_VMD
14 Fog_VMD
15 Ambient_Occlusion
16 | Ambient_Color 0.8 0.8 0.8
17 | Rescale_Direct 0.4
18 Samples 12
19 End_Shader_Mode
20 Camera
21 | Projection Orthographic
22 | Zoom 0.333333
23 | Aspectratio 1
24 | Antialiasing 12
25 | Raydepth 50
26 | Center 0 0 -2
27 | Viewdir -0 -0 2
28 | Updir 0 1 -0
29 End_Camera
30 Directional_Light Direction 0.1 -0.1 1 Color 1 1 1
31 Directional_Light Direction -1 -2 0.5 Color 1 1 1
32
33 Background 1 1 1
34 Fog Exp2 Start 0 End 10 Density 0.32 Color 1 1 1
35 # Mol[0] Rep[0] NewCartoon
36 VertexArray Numverts 16930
37
38 Coords
39 -0.171524 0.756148 0.251898
```

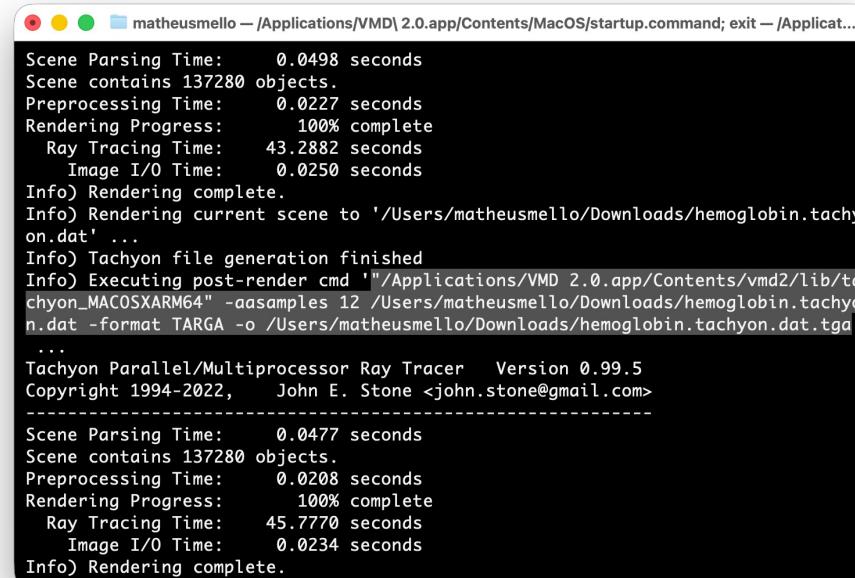
Ln 33, Col 17 Spaces: 2 UTF-8 LF Plain Text Prettier

.dat file: configures the scene

Some things we can change:

- Resolution > 500 500
- Fog | Density 0.32 > 0.30

VMD terminal



A screenshot of a Mac OS X terminal window titled "matheusmello — /Applications/VMD 2.0.app/Contents/MacOS/startup.command; exit — /Applicat...". The window displays the output of a rendering command. It shows the scene parsing time, preprocessing time, rendering progress (100% complete), ray tracing time, and image I/O time. The output also includes information about the Tachyon Parallel/Multiprocessor Ray Tracer version and copyright details. The terminal interface has a dark theme with light-colored text.

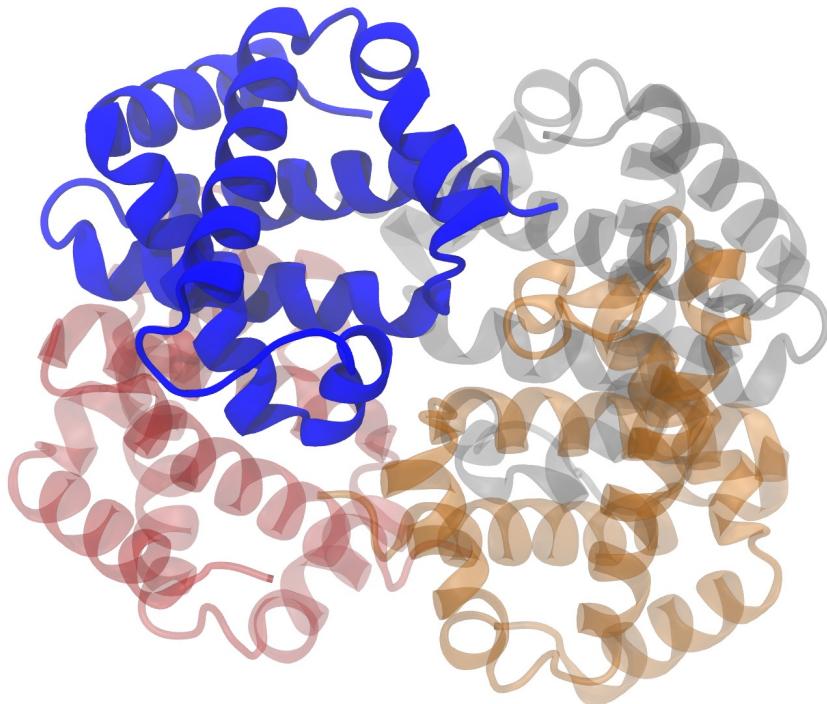
```
Scene Parsing Time: 0.0498 seconds
Scene contains 137280 objects.
Preprocessing Time: 0.0227 seconds
Rendering Progress: 100% complete
Ray Tracing Time: 43.2882 seconds
Image I/O Time: 0.0250 seconds
Info) Rendering complete.
Info) Rendering current scene to '/Users/matheusmello/Downloads/hemoglobin.tachyon.dat' ...
Info) Tachyon file generation finished
Info) Executing post-render cmd '/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64' -aasamples 12 /Users/matheusmello/Downloads/hemoglobin.tachyon.dat -format TARGA -o /Users/matheusmello/Downloads/hemoglobin.tachyon.dat.tga'
...
Tachyon Parallel/Multiprocessor Ray Tracer Version 0.99.5
Copyright 1994-2022, John E. Stone <john.stone@gmail.com>
-----
Scene Parsing Time: 0.0477 seconds
Scene contains 137280 objects.
Preprocessing Time: 0.0208 seconds
Rendering Progress: 100% complete
Ray Tracing Time: 45.7770 seconds
Image I/O Time: 0.0234 seconds
Info) Rendering complete.
```

} Copy rendering command

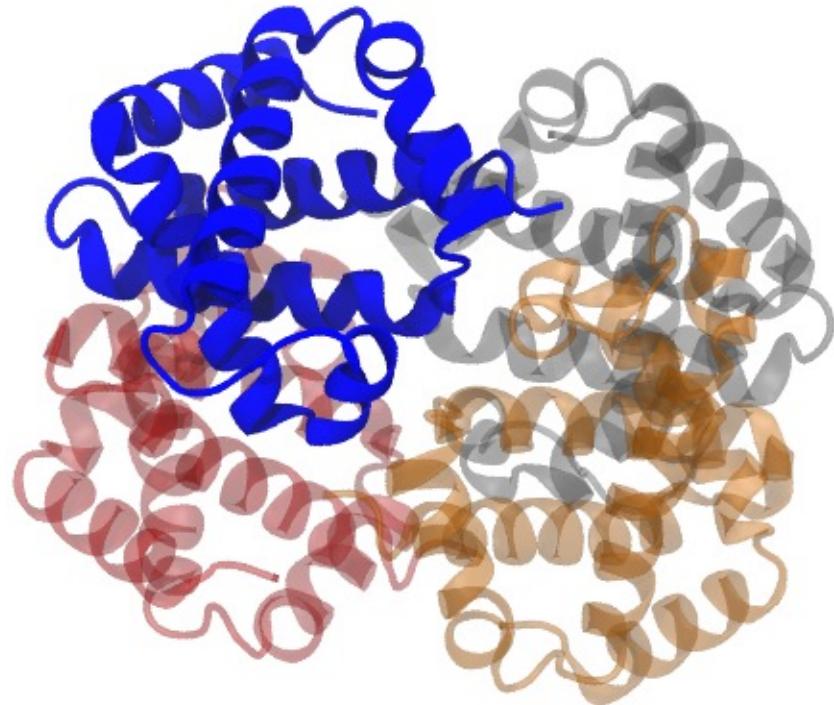
version 2.0.0

# Rendering images

Tachyon



edited .dat file



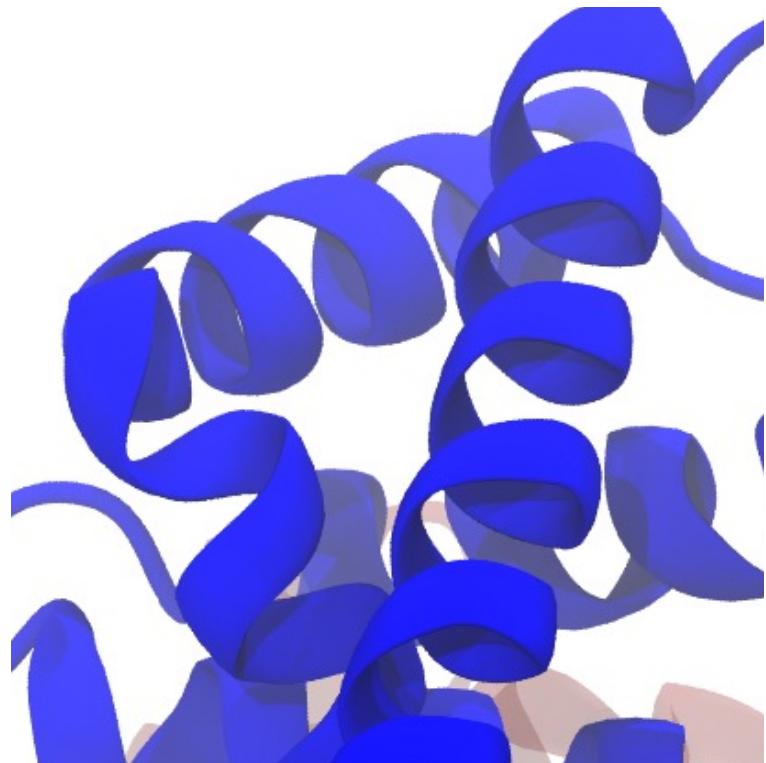
On a new terminal

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -aasamples 12  
hemoglobin.tachyon.edited.dat -format TARGA -o hemoglobin.tachyon.edited.dat.tga
```

version 2.0.0

# Rendering images

Tachyon



edited .dat file



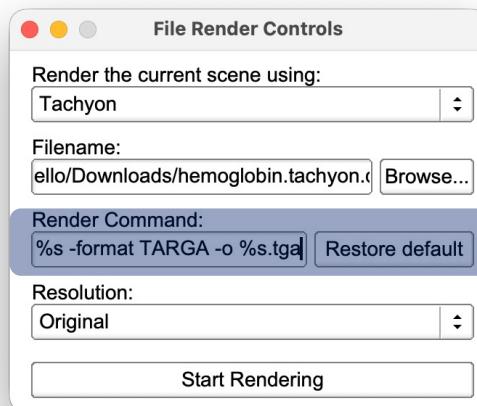
On a new terminal

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -aasamples 12  
hemoglobin.tachyon.edited.dat -format TARGA -o hemoglobin.tachyon.edited.dat.tga
```

version 2.0.0

# Rendering images

We can also change the rendering command:



Default command:

```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64"  
-aasamples 12 %s -format TARGA -o %s.tga
```

We can add:

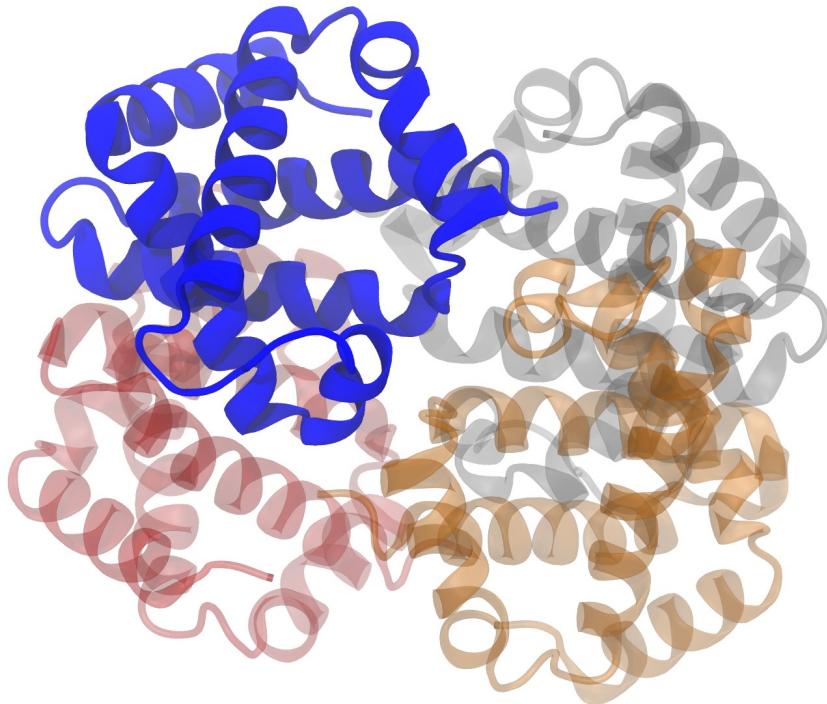
```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -  
aasamples 12 %s -fullshade -auto_skylight 1.4 -format TARGA -o %s.tga
```



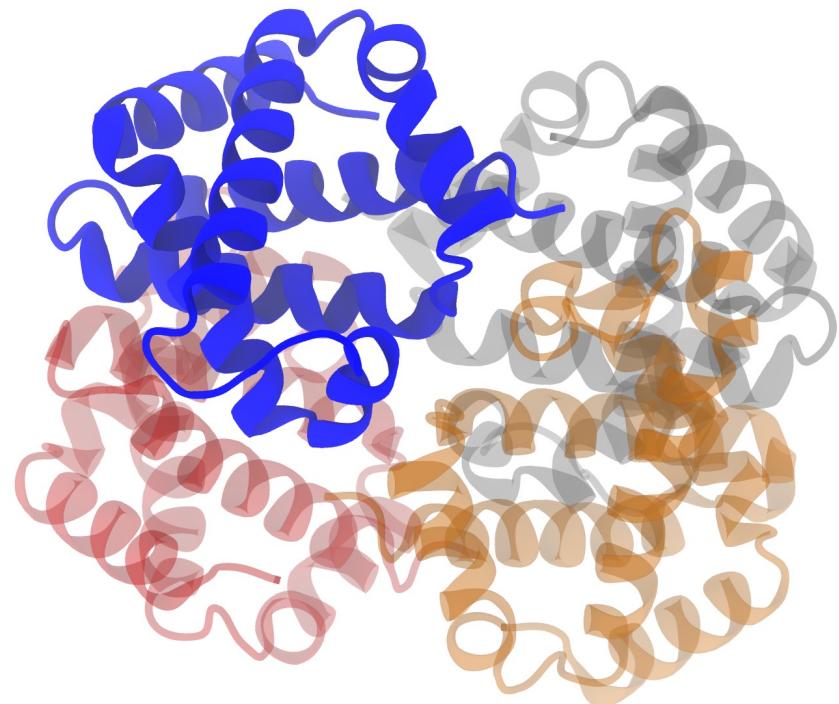
It will take considerably longer to render

# Rendering images

Tachyon

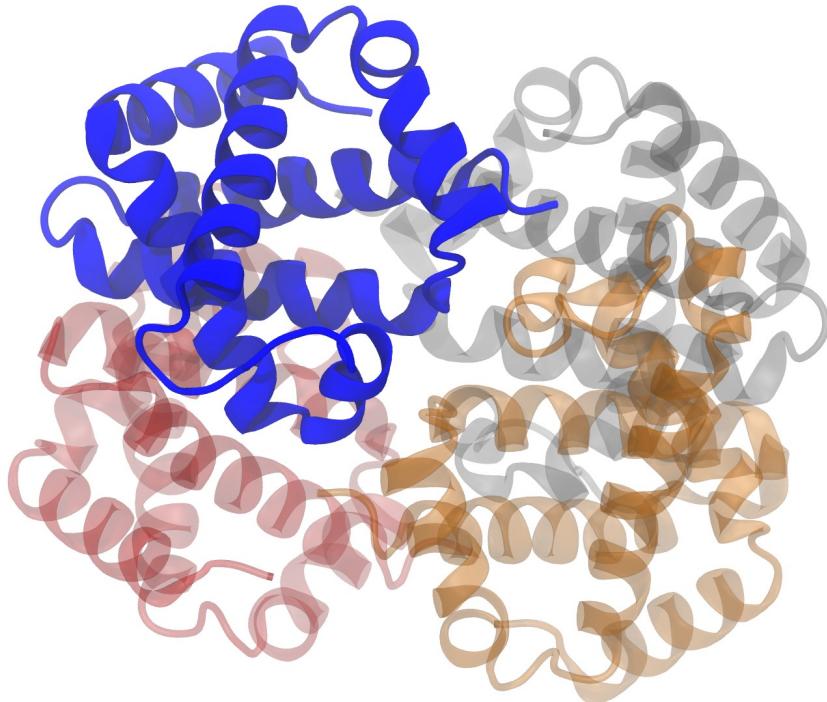


“Fancy” Tachyon

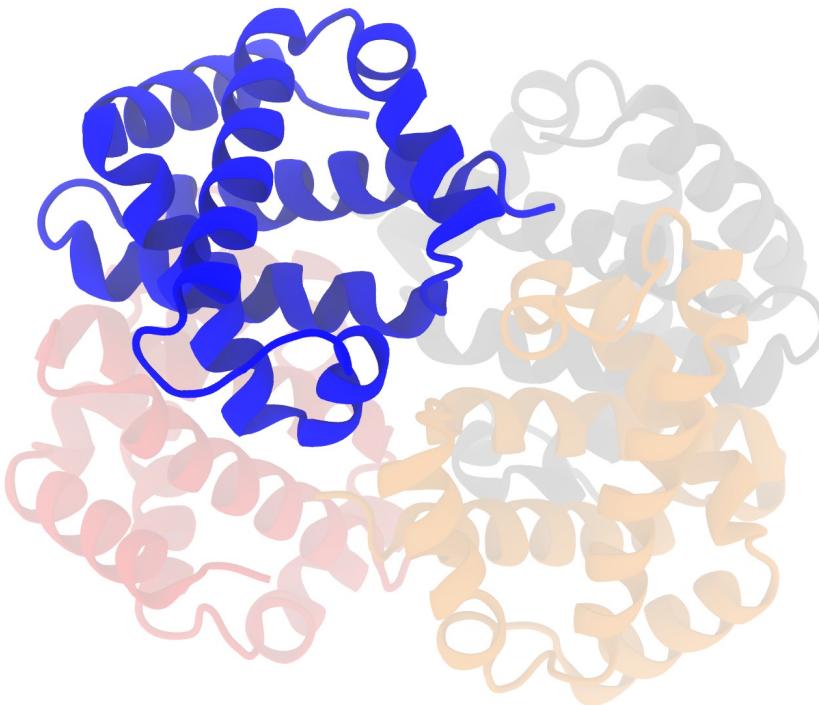


# Rendering images

Tachyon

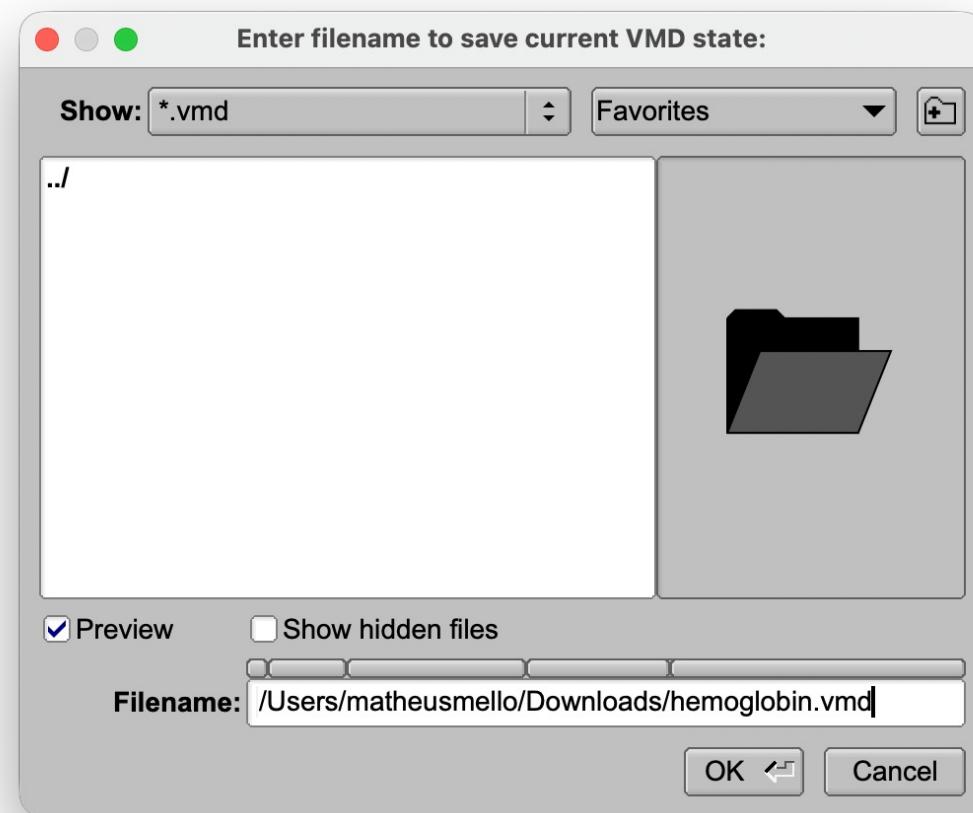
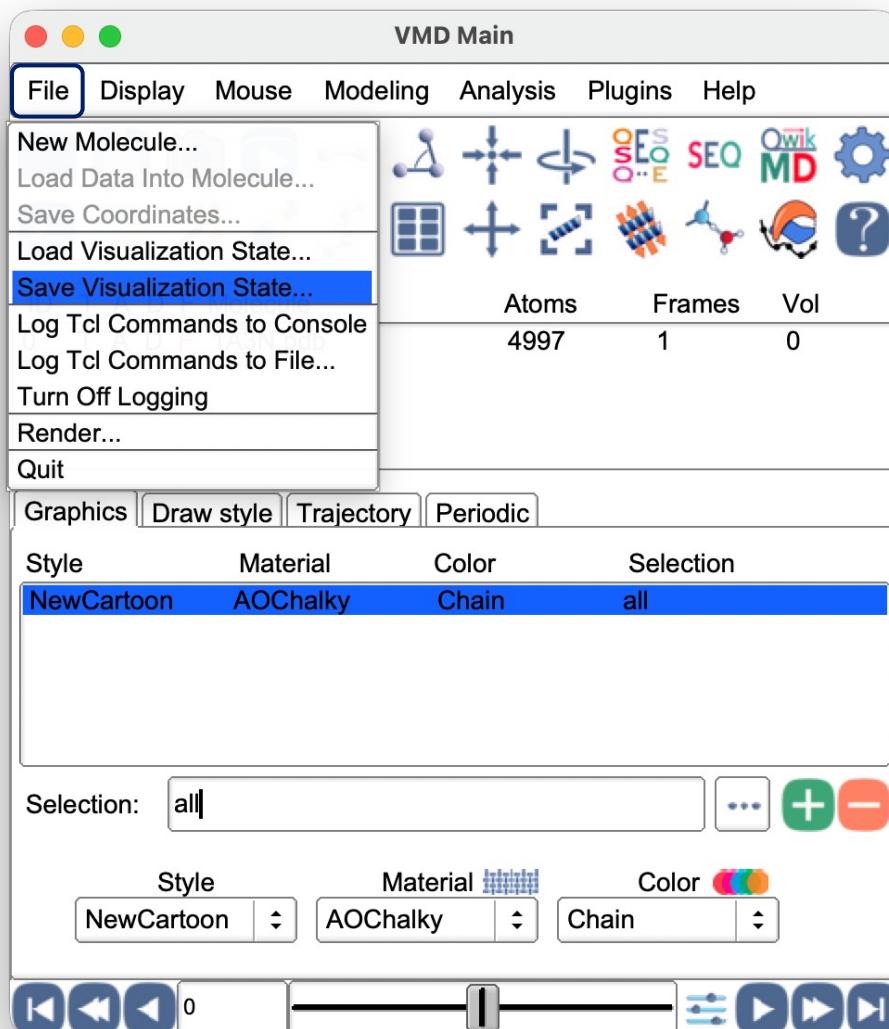


“Fancy” Tachyon



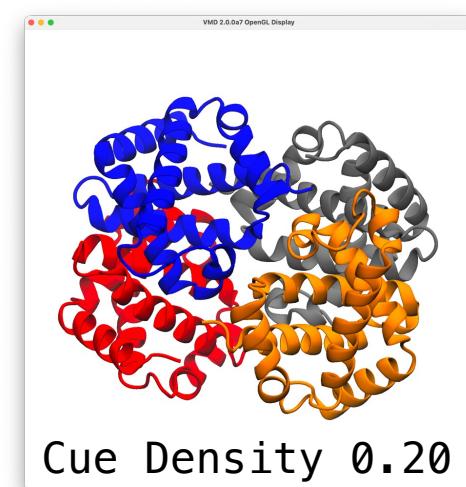
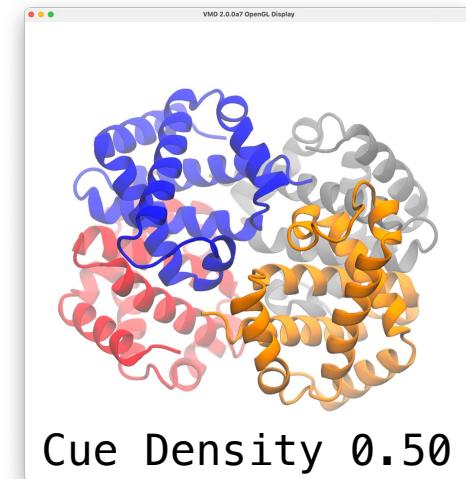
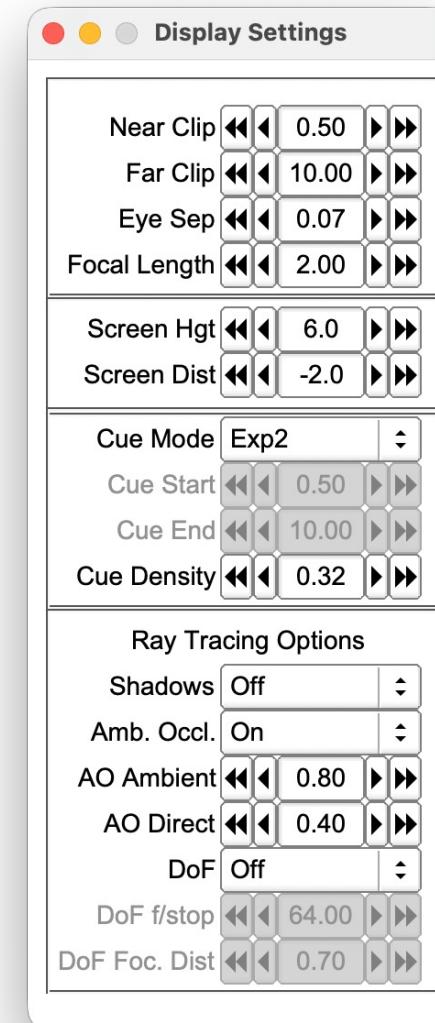
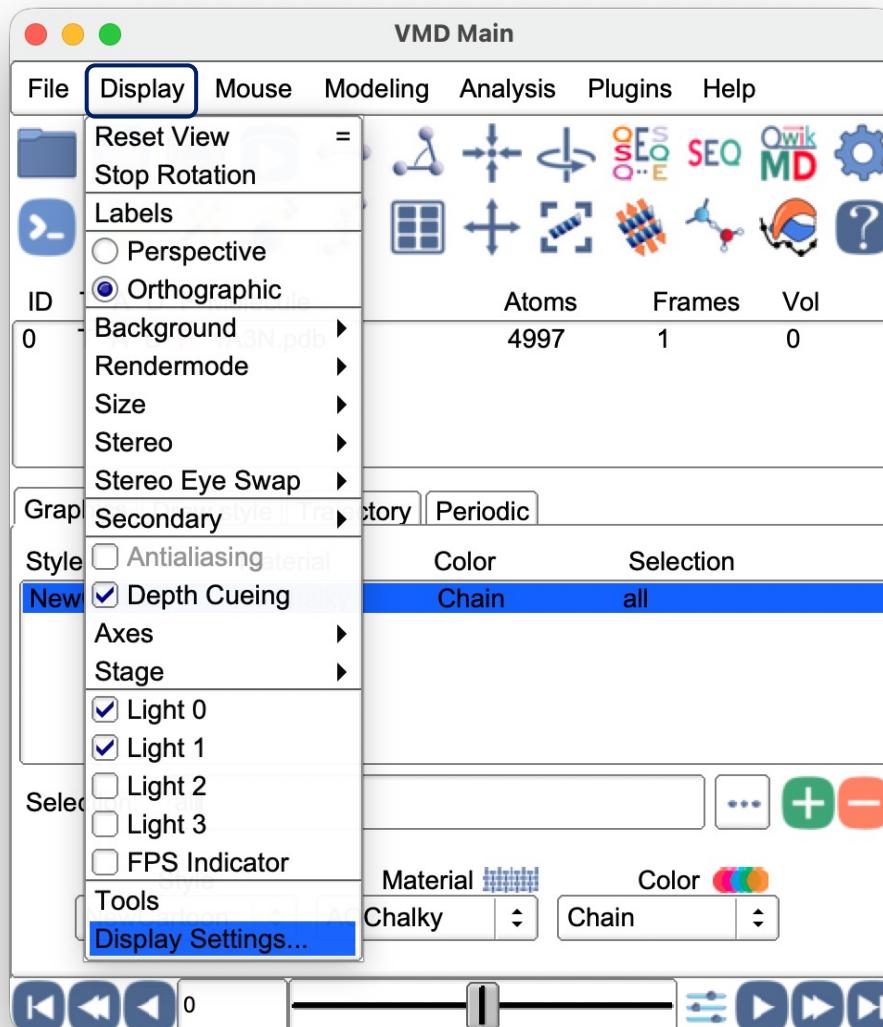
For transparent objects, we can add  
`-trans_max_surfaces 1`

# Saving current scene



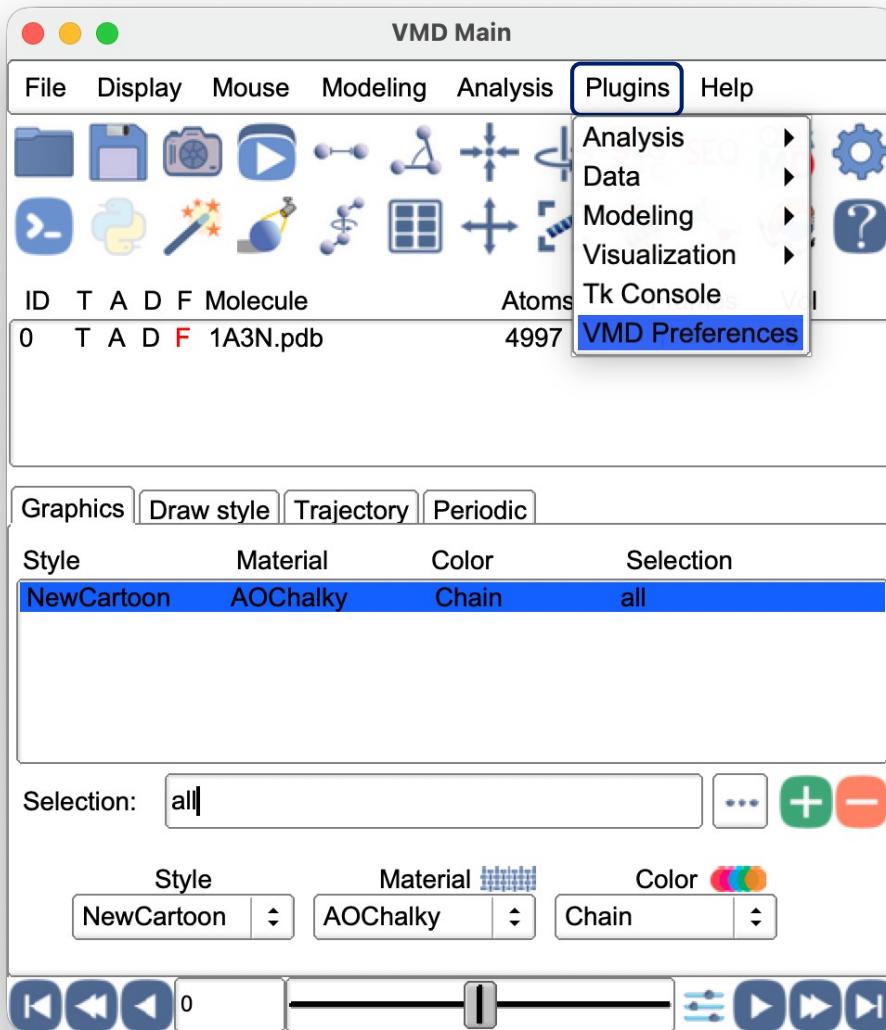
Useful to save the scene of a presentation or publication figure

# Advanced options

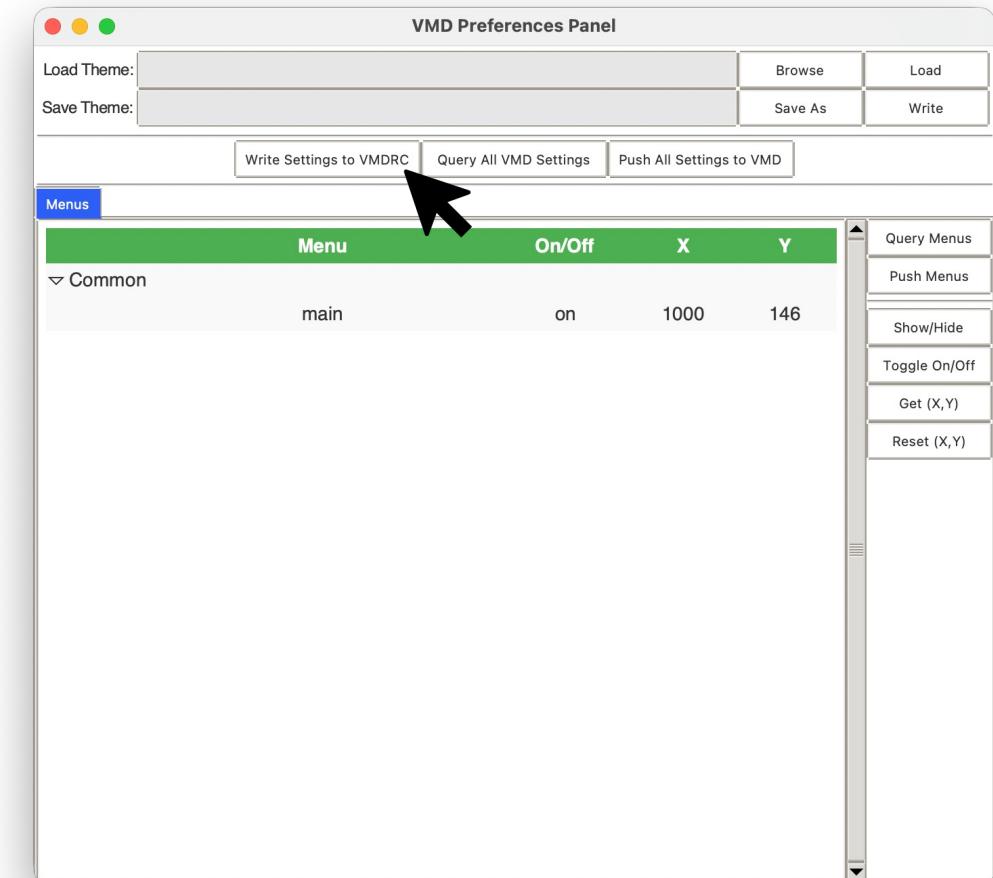


version 2.0.0

# Advanced options

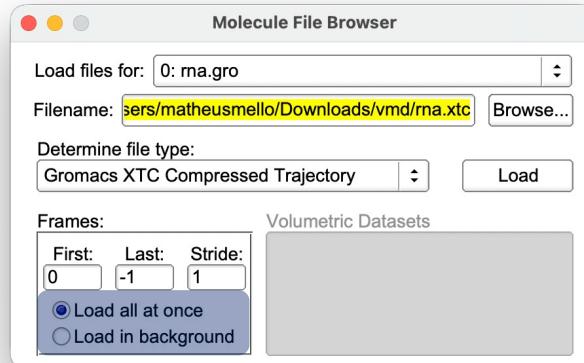
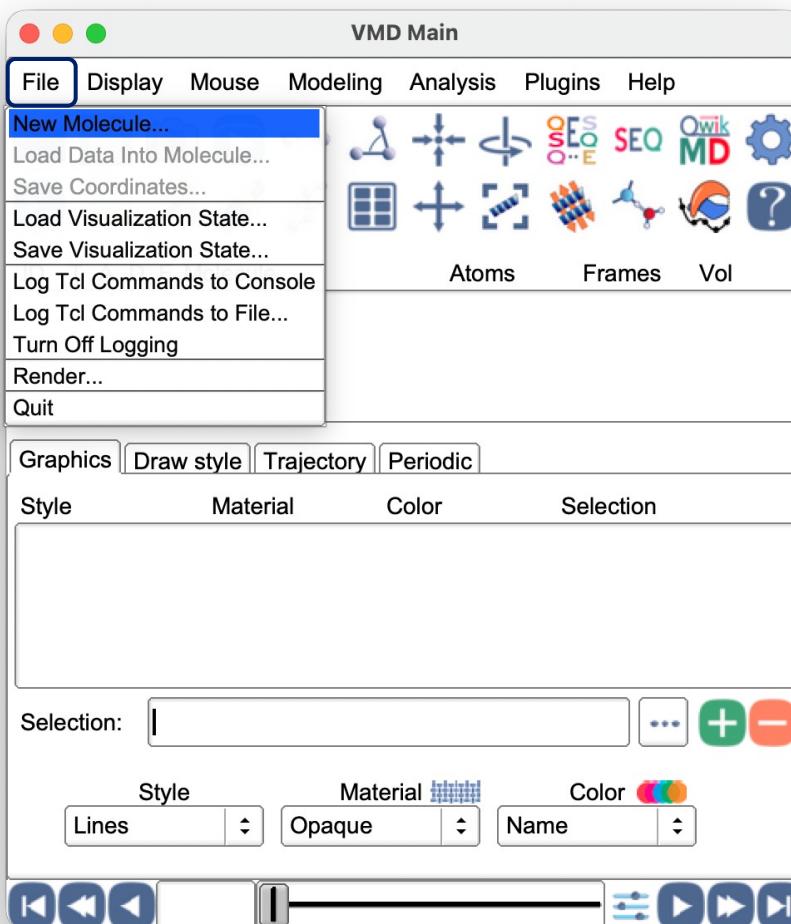


Save current settings, to apply every time VMD opens:



# Managing trajectories

Load RNA model (rna.gro) and trajectory (rna.xtc)



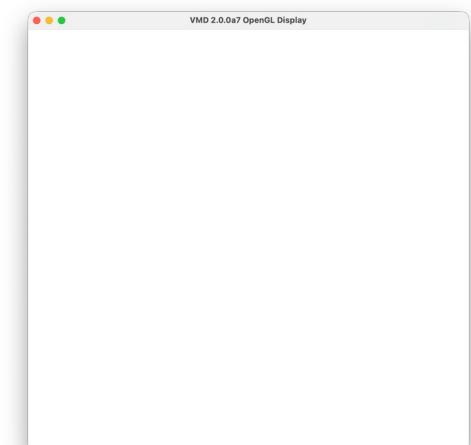
) The trajectory file is loaded on top of the topology file  
]) Load all at once loads faster, especially for larger systems



Note that the molecule leaves the field of view

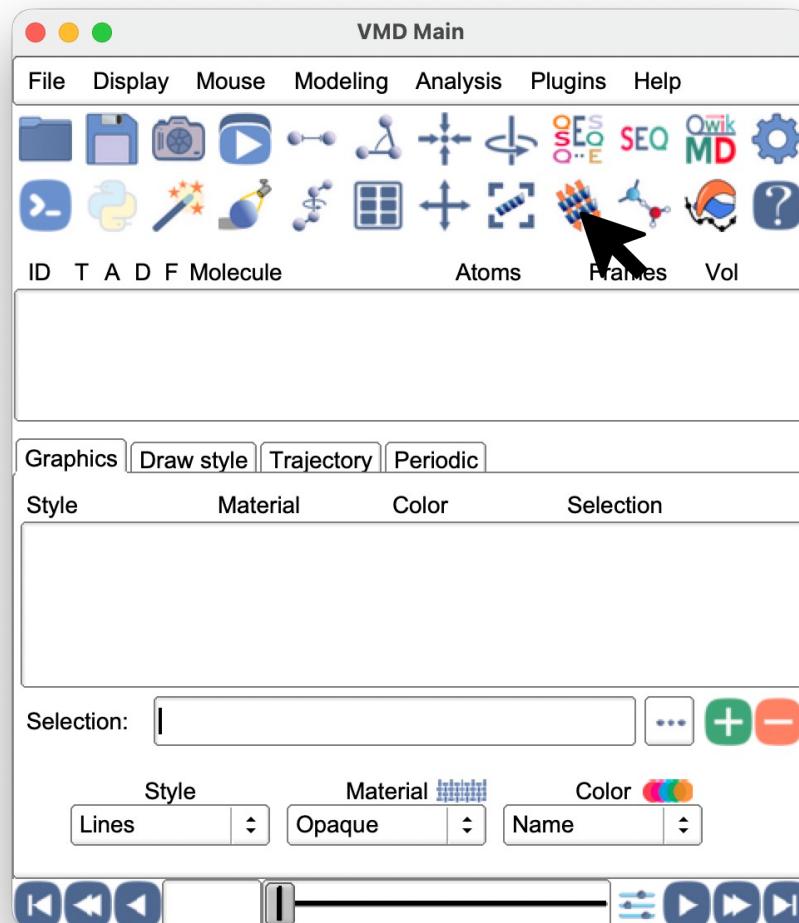
Solutions:

- press '=' to reset view
- align trajectory to first frame

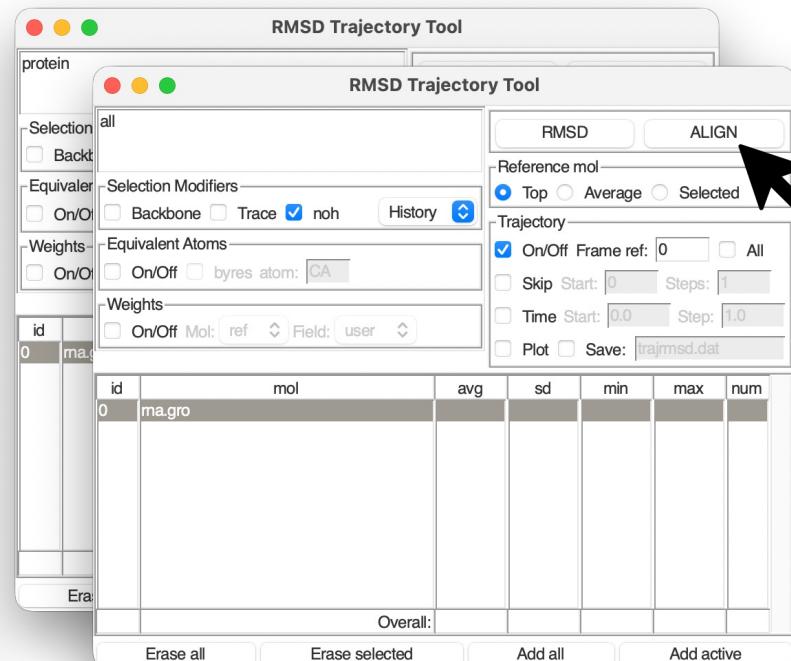


# Aligning trajectories

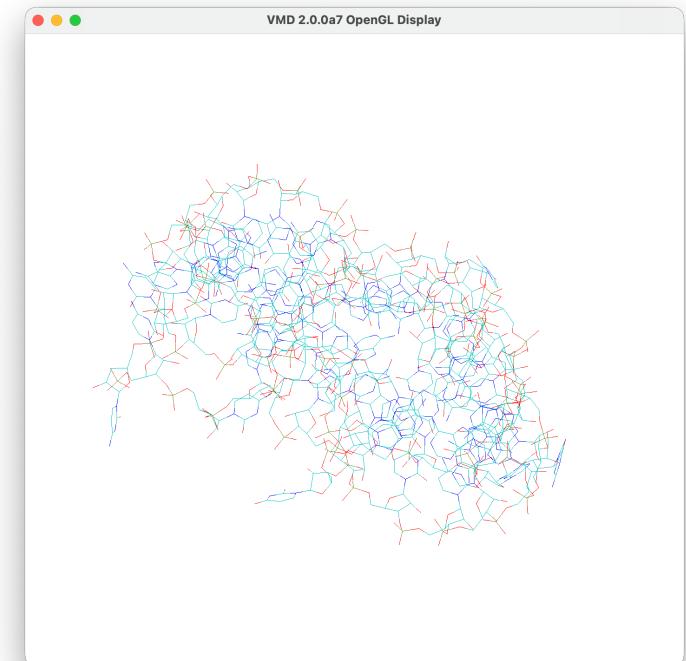
Open RMSD Trajectory tool



Change selection and align



Reset view (=)

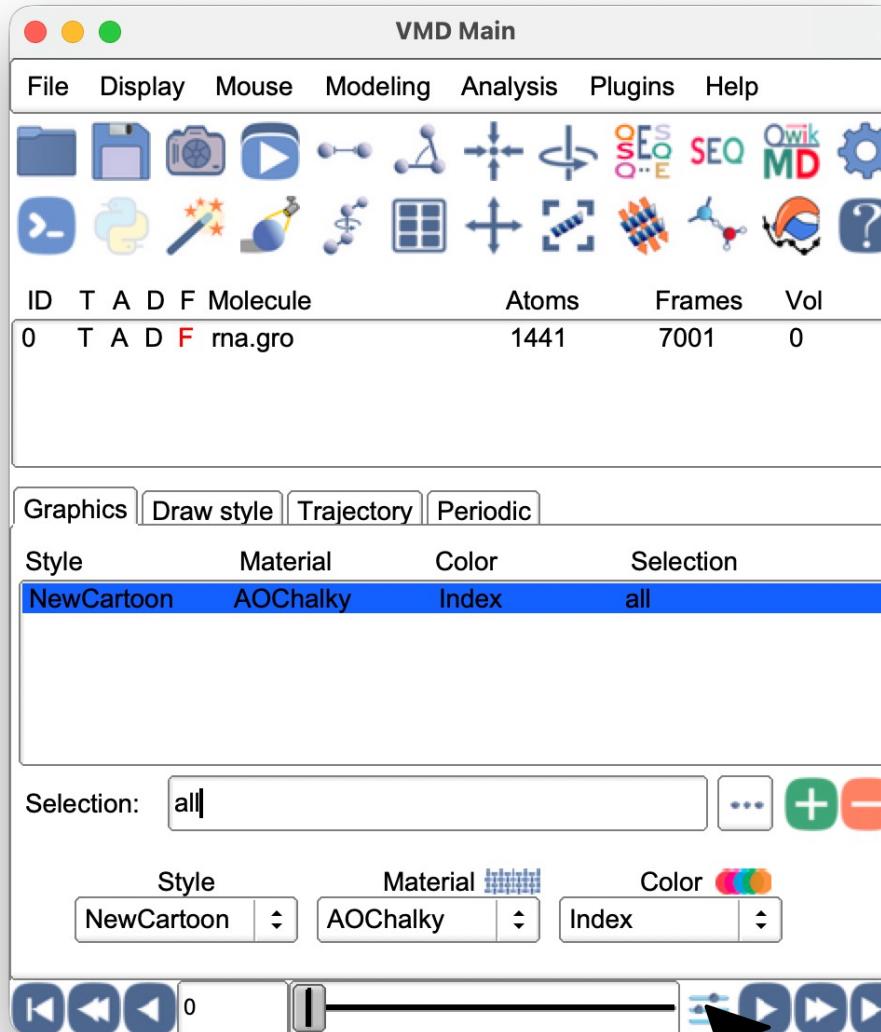


Try a custom selection and explore a representation that you like!

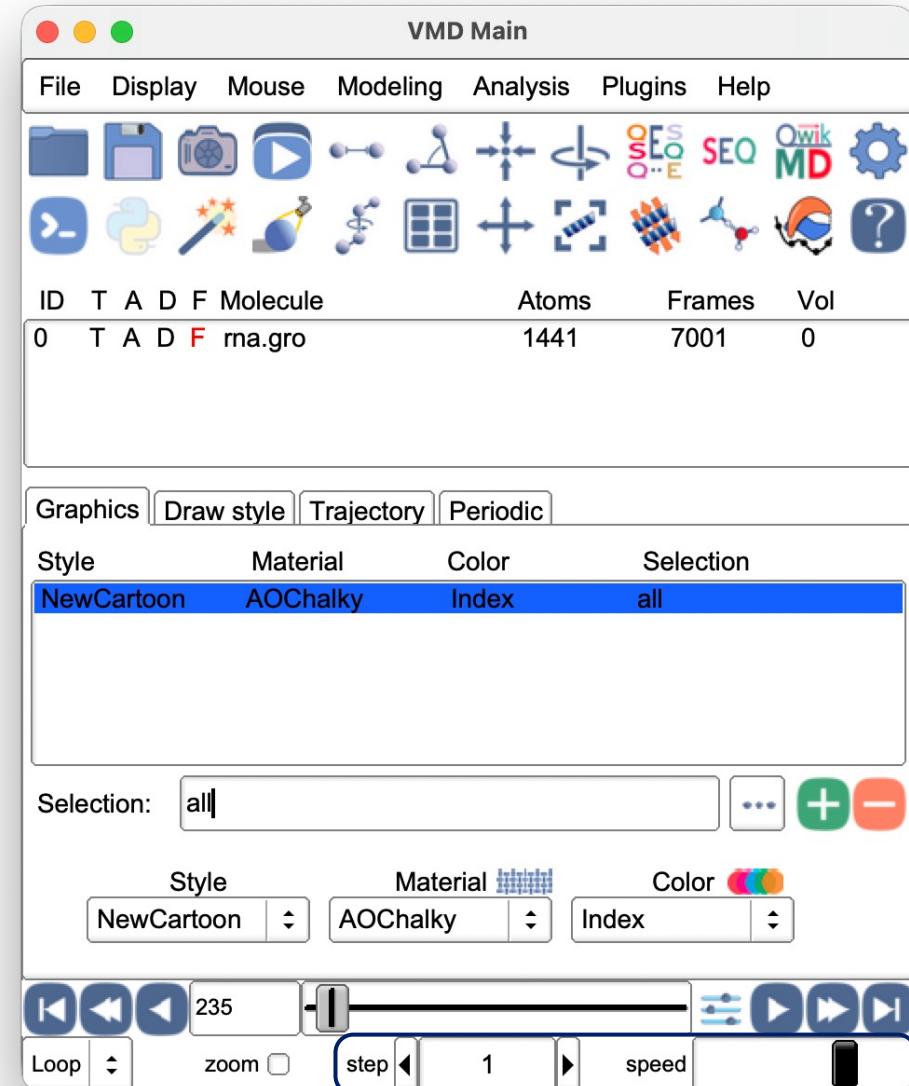
Alternatively : Extensions > Analysis > RMSD Trajectory Tool

version 2.0.0

# Managing trajectories

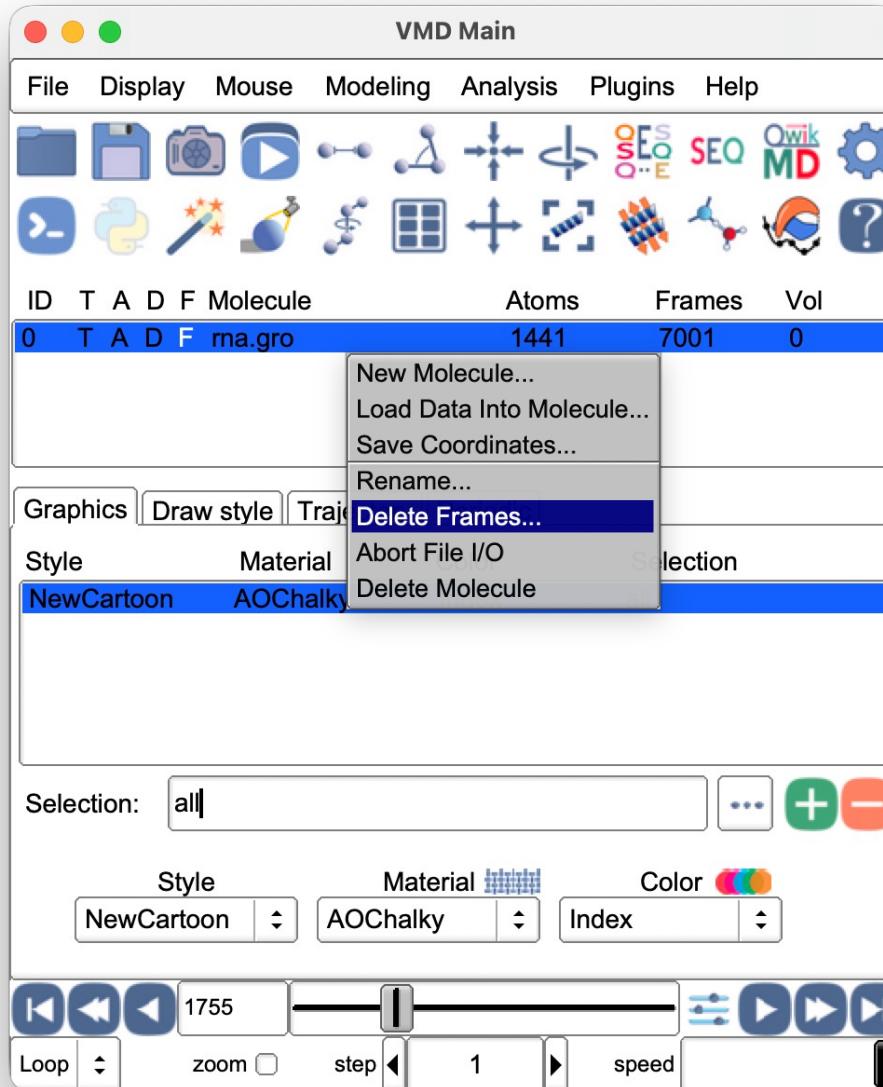


Skip to last frame  
Next frame  
Play forward

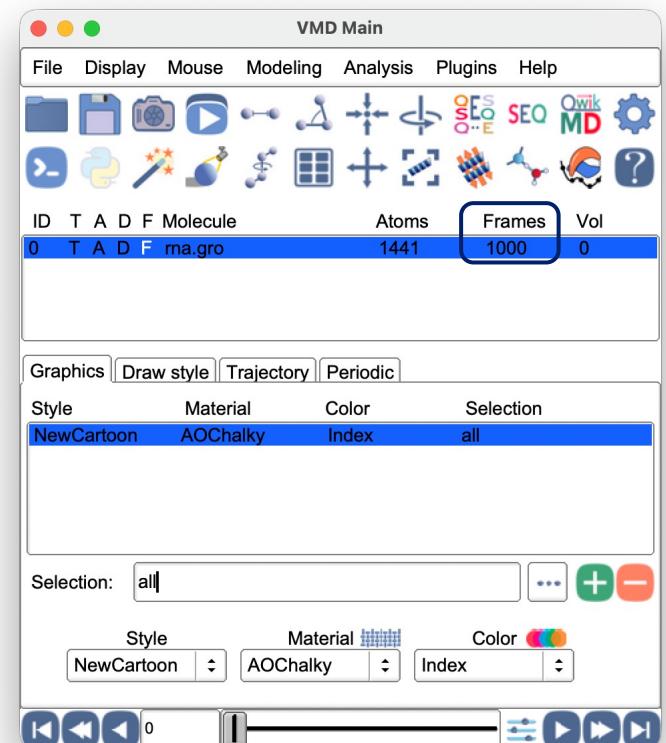
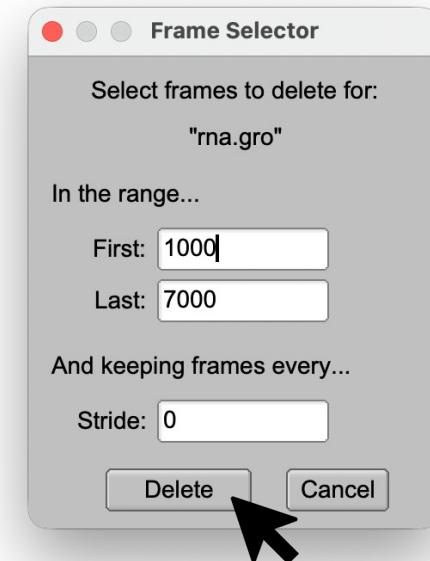


version 2.0.0

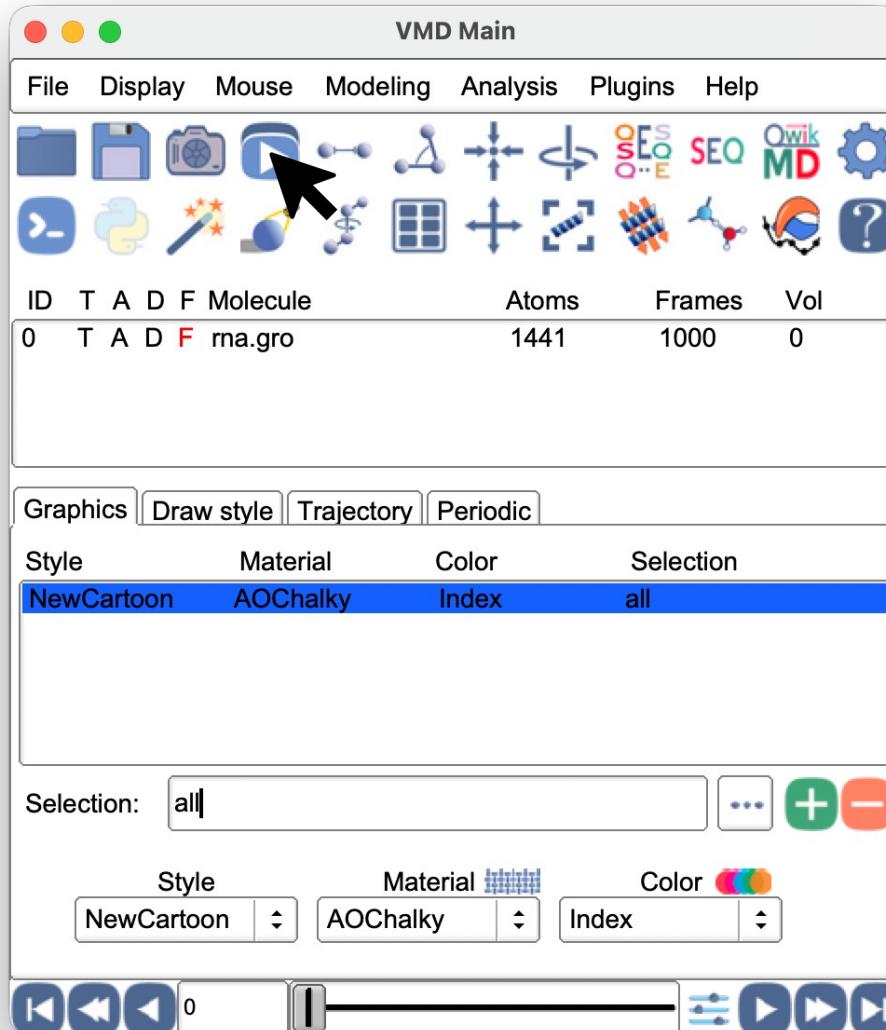
# Managing trajectories



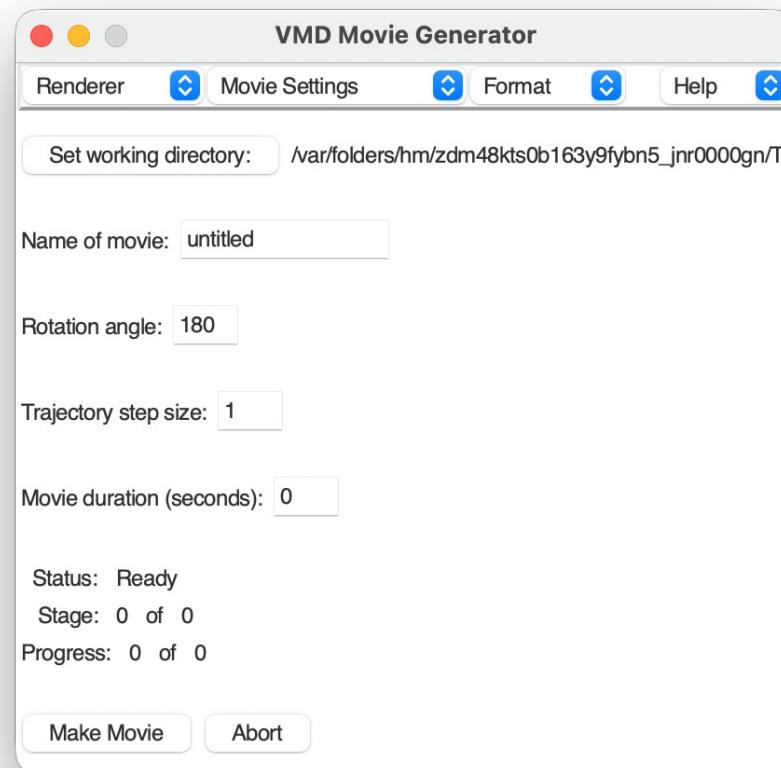
The trajectory is quite long!  
Let's keep only the first 1,000 frames.



# Rendering videos



Alternatively: Extensions > Visualization  
(version 1.9.4)  
> Movie Maker

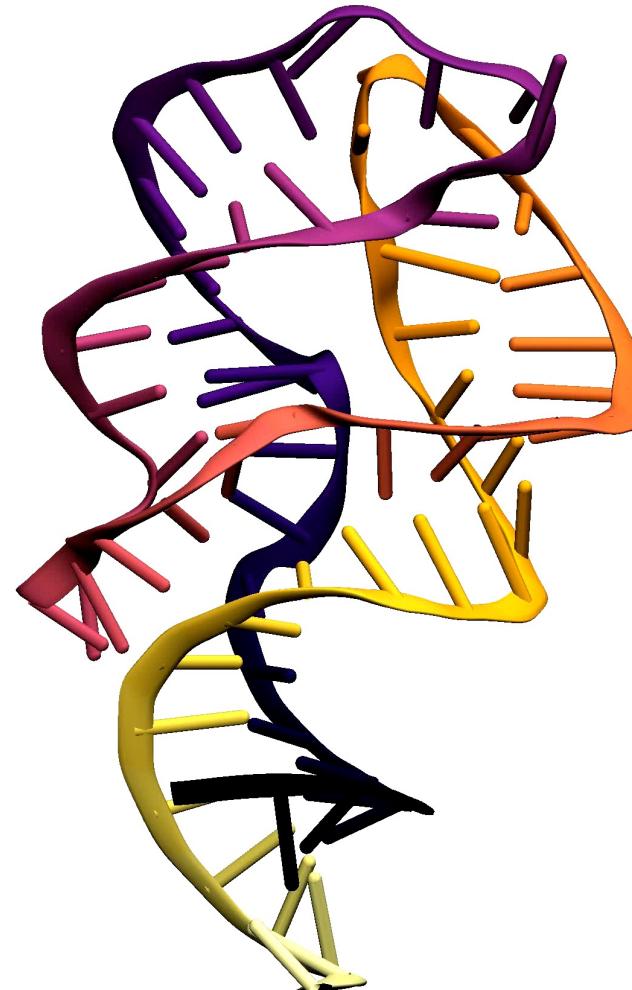


} Set the proper directory  
Name your movie

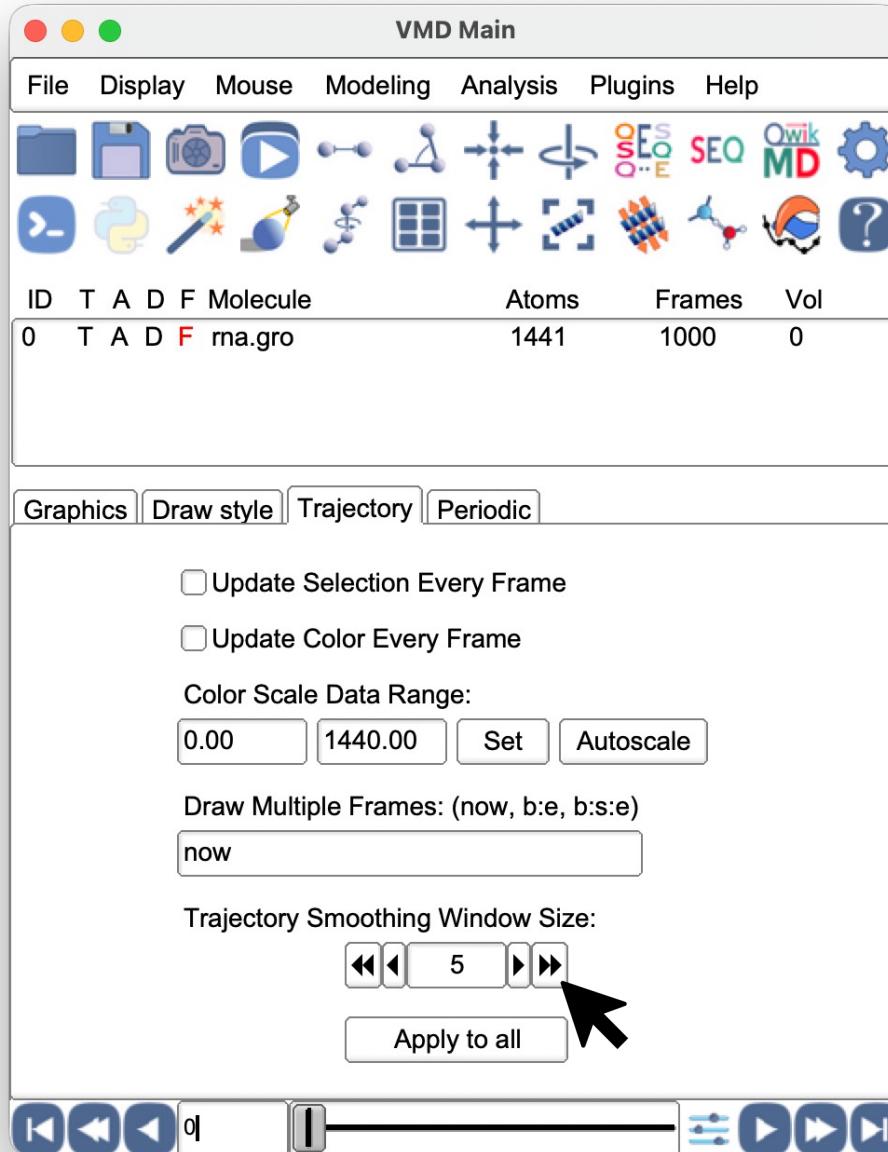
version 2.0.0

# Rendering videos

Our results so far...

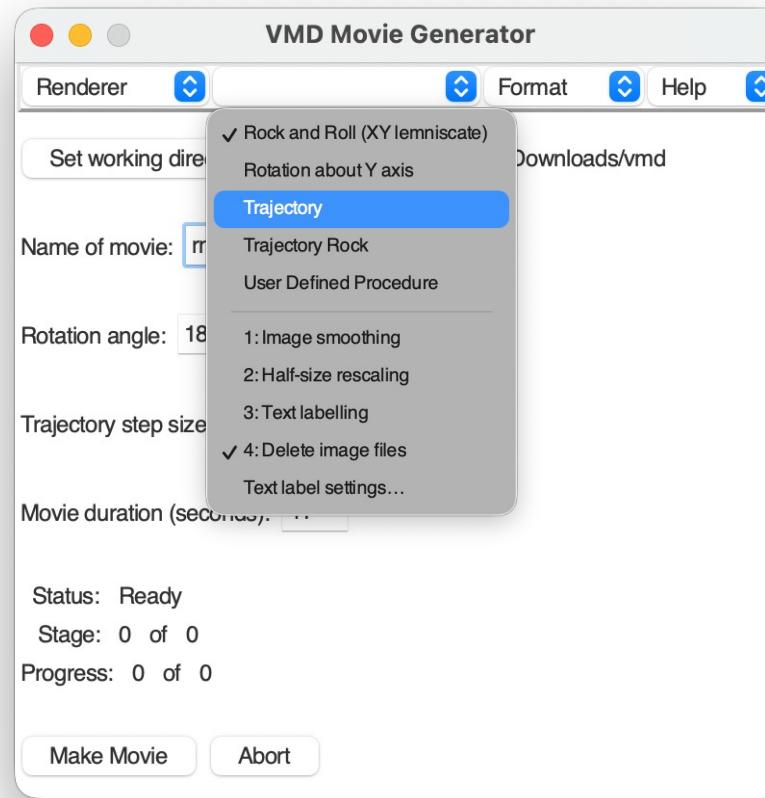


# Rendering videos



## Change Movie Settings to Trajectory

You can also change the renderer to Tachyon, but the rendering time will increase significantly



# Rendering videos

Smoothing = 5



Smoothing = 0



# Questions?

