



Introduction to VMD

Using the GUI effectively

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Agenda



Basic UI
elements



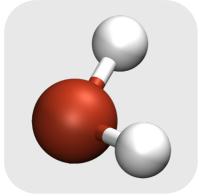
Rendering
images



Rendering
videos

Why use VMD?

Molecular visualization available software



VMD

- Analysis and visualization of time-dependent data (trajectories)
- Integrates with NAMD
- Powerful scripting with Tcl
- Available plugins/extensions for MD analysis



PyMOL

- User-friendly interface
- Best for a single structure
- Strong renderings with little settings



ChimeraX

- Analysis and visualization of cryo-EM maps
- Also strong in still structures
- Strong modeling tools

VMD 2.0.0 – alpha version



We will use the pre-release
VMD 2.0.0 alpha test version



As VMD 2.0.0a7 is a recent release (August 2025), it may still contain some bugs.

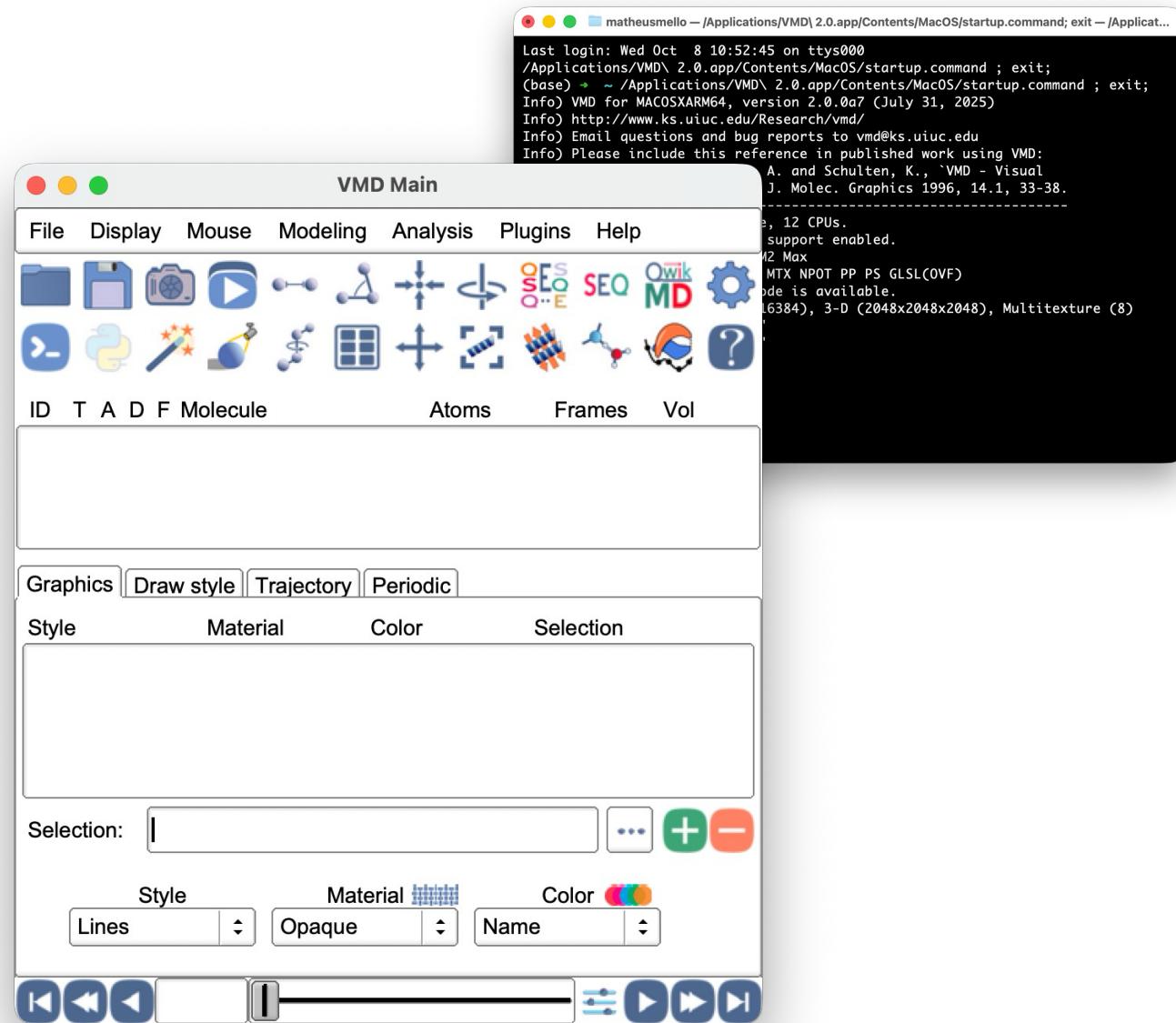
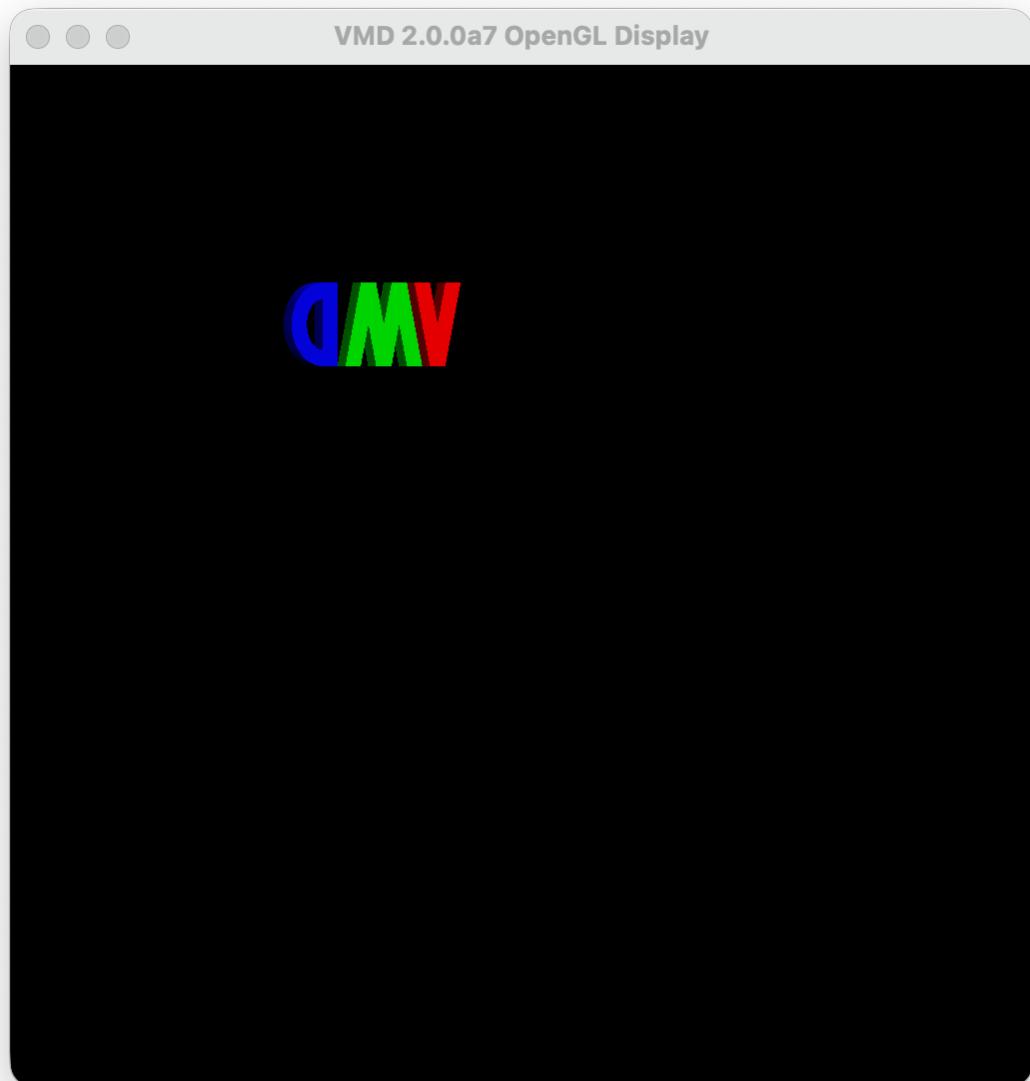


Bug reports, comments, and suggestions can be sent to
vmd@ks.uiuc.edu



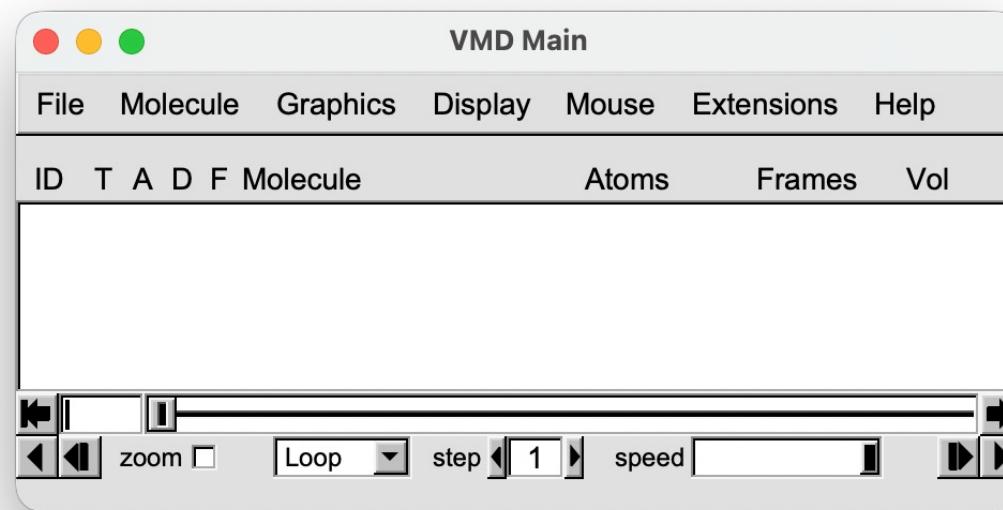
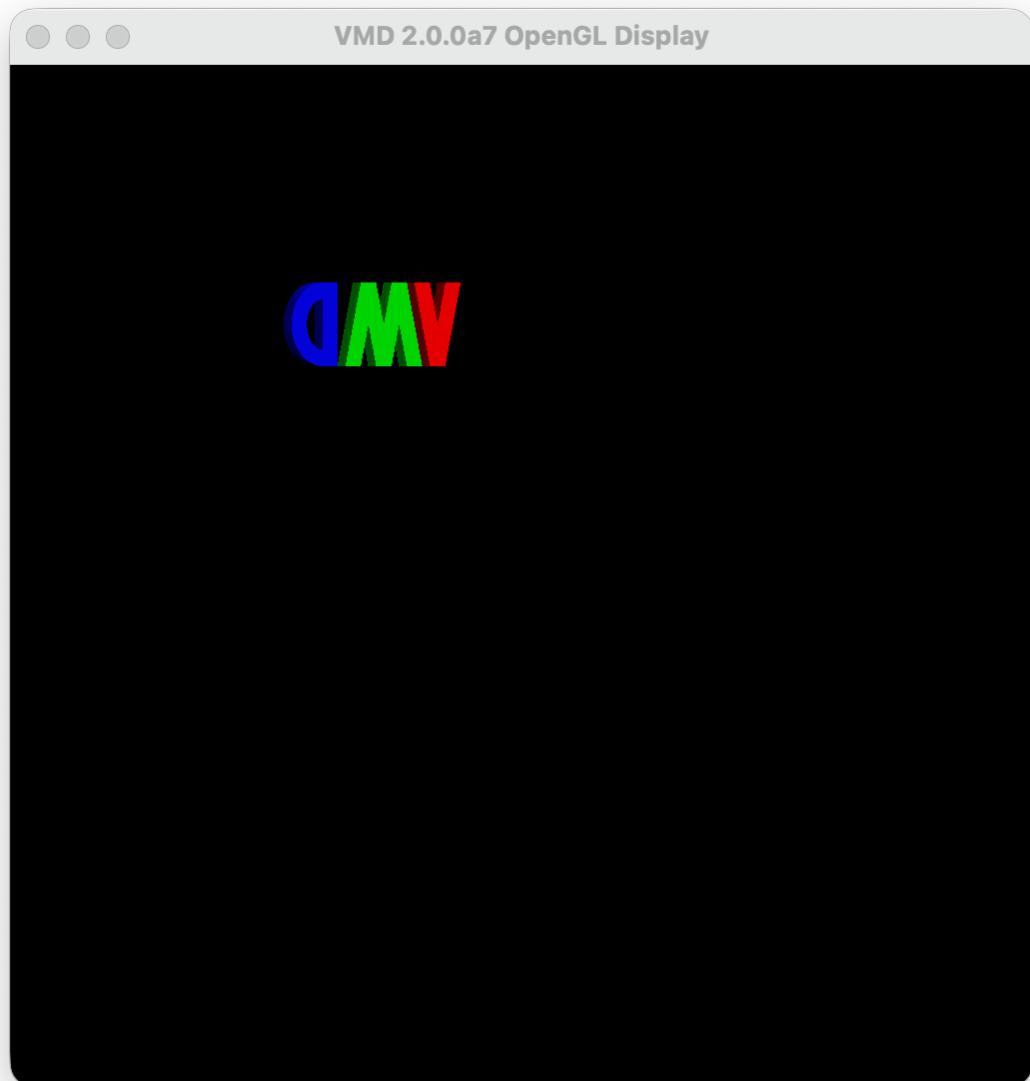
Using previous VMD versions will not affect your ability to participate

Opening VMD



version 2.0.0

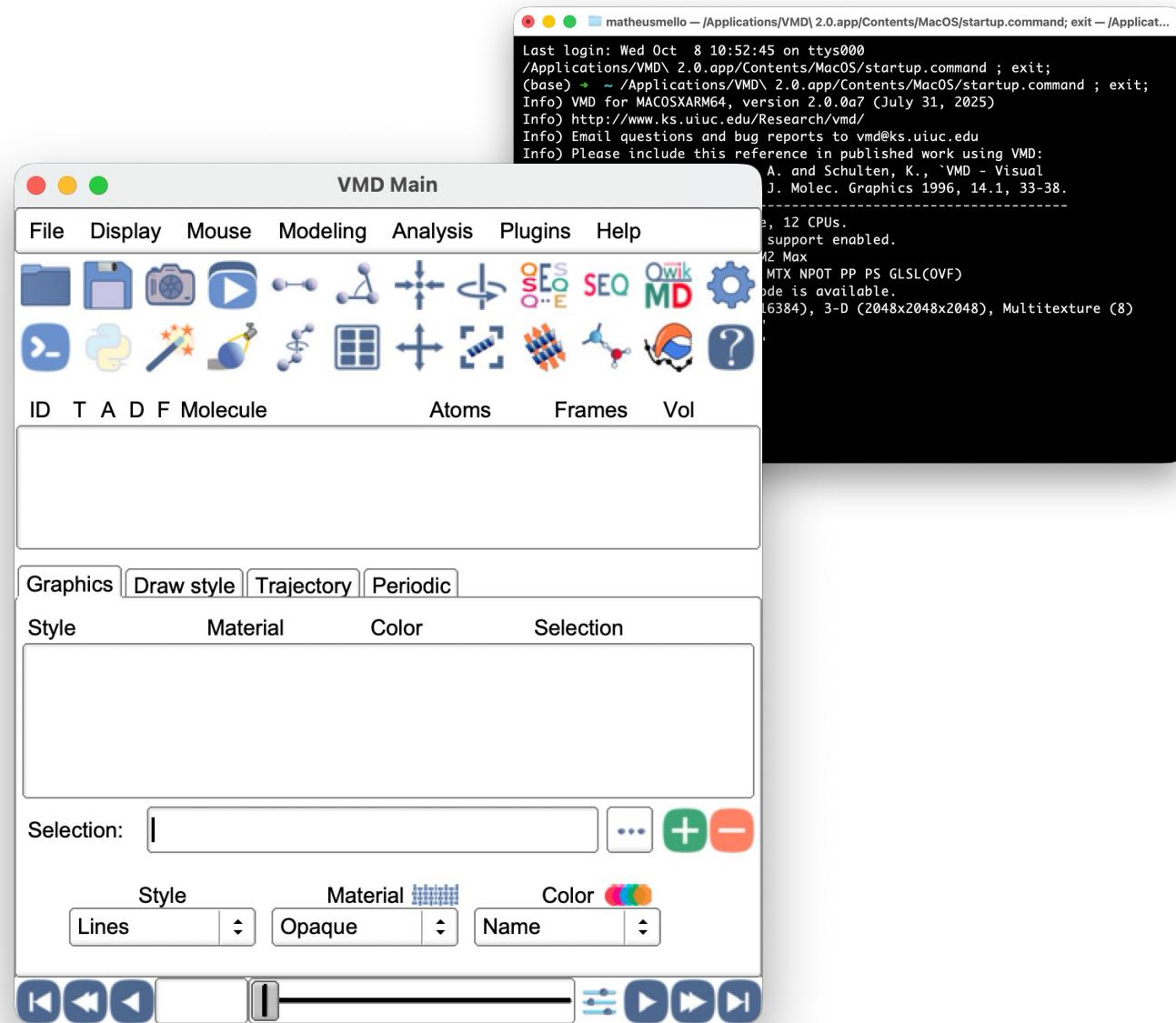
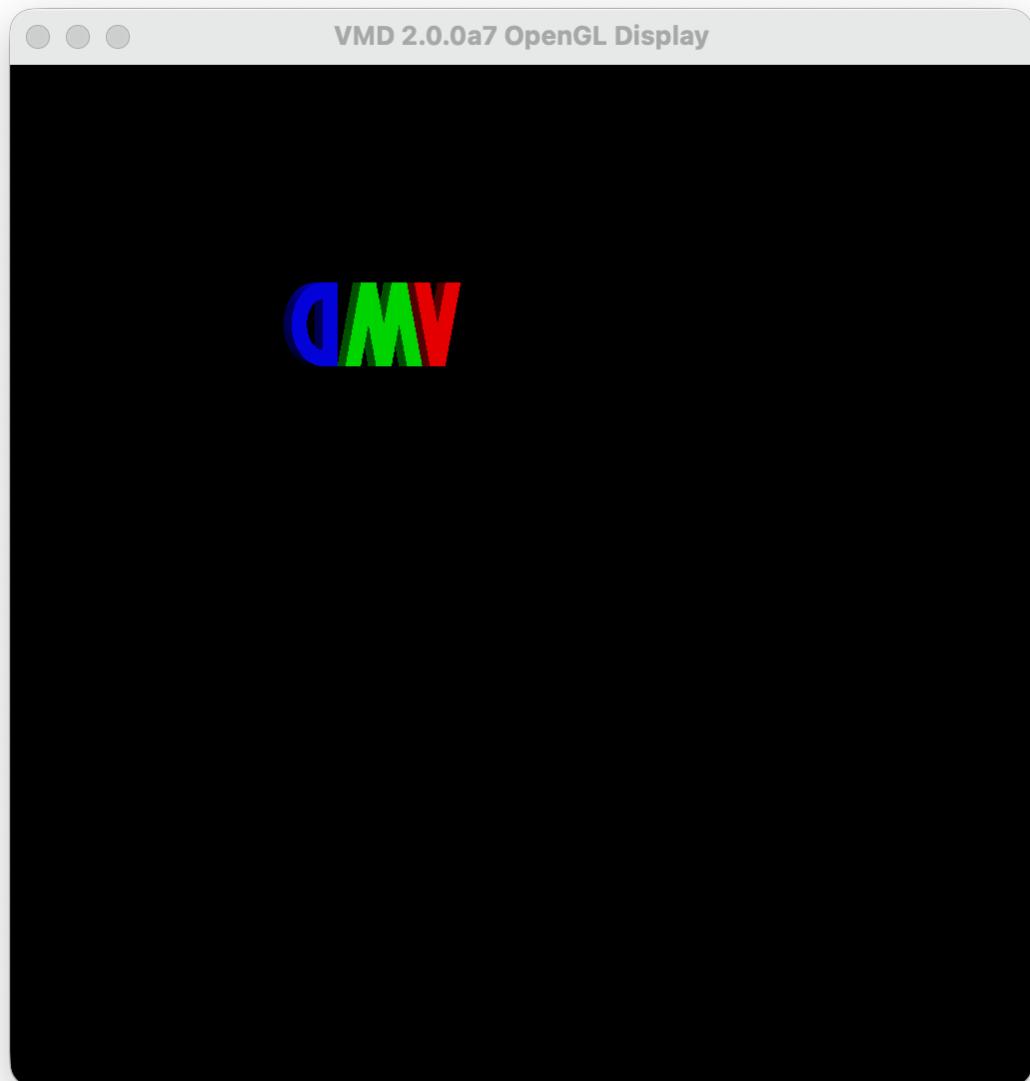
Opening VMD



```
matheusmello ~ /Applications/VMD\ 2.0.app/Contents/MacOS/startup.command; exit ~ /Appl...
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 >
```

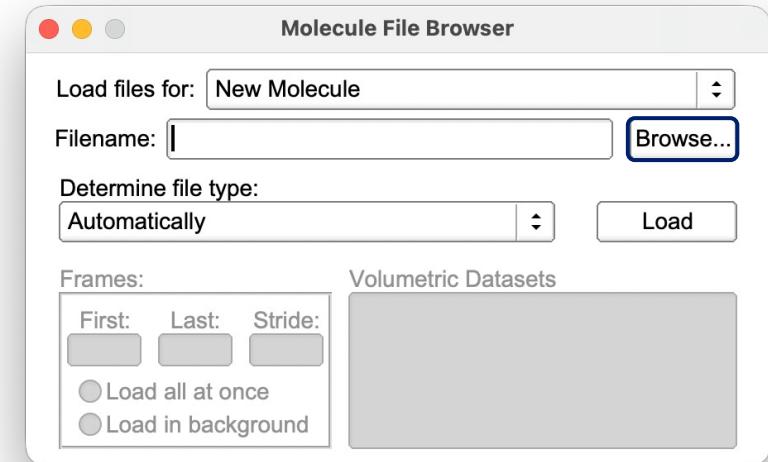
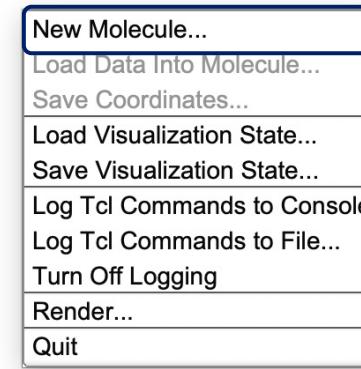
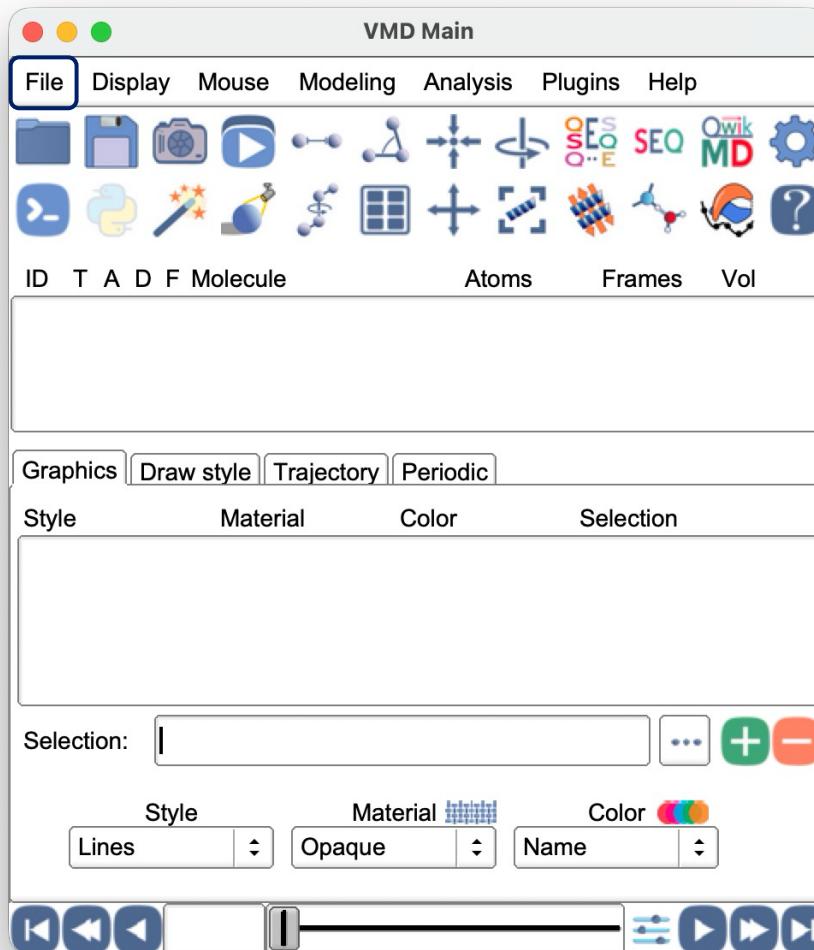
version 1.9.4

Opening VMD



version 2.0.0

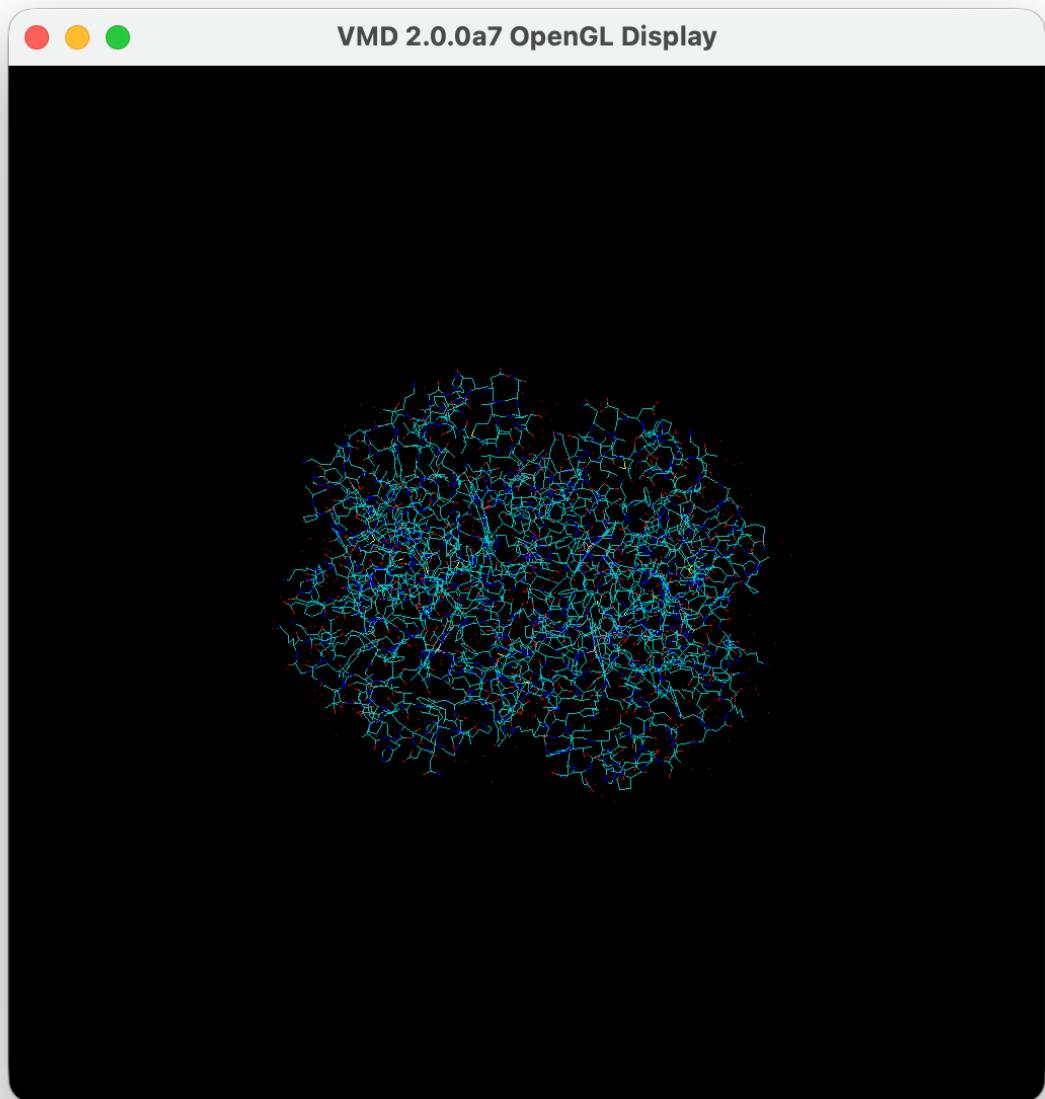
Loading a molecule



Download PDB
1a3n.pdb

rcsb.org/structure/1A3N

Loading a molecule



VMD Main

File Display Mouse Modeling Analysis Plugins Help

File Manager: Open, Save, Camera, Play, Selection Tools, SEQ, MD, Plugins, Python, Script, Grid, Molecule, Atoms, Frames, Volume

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

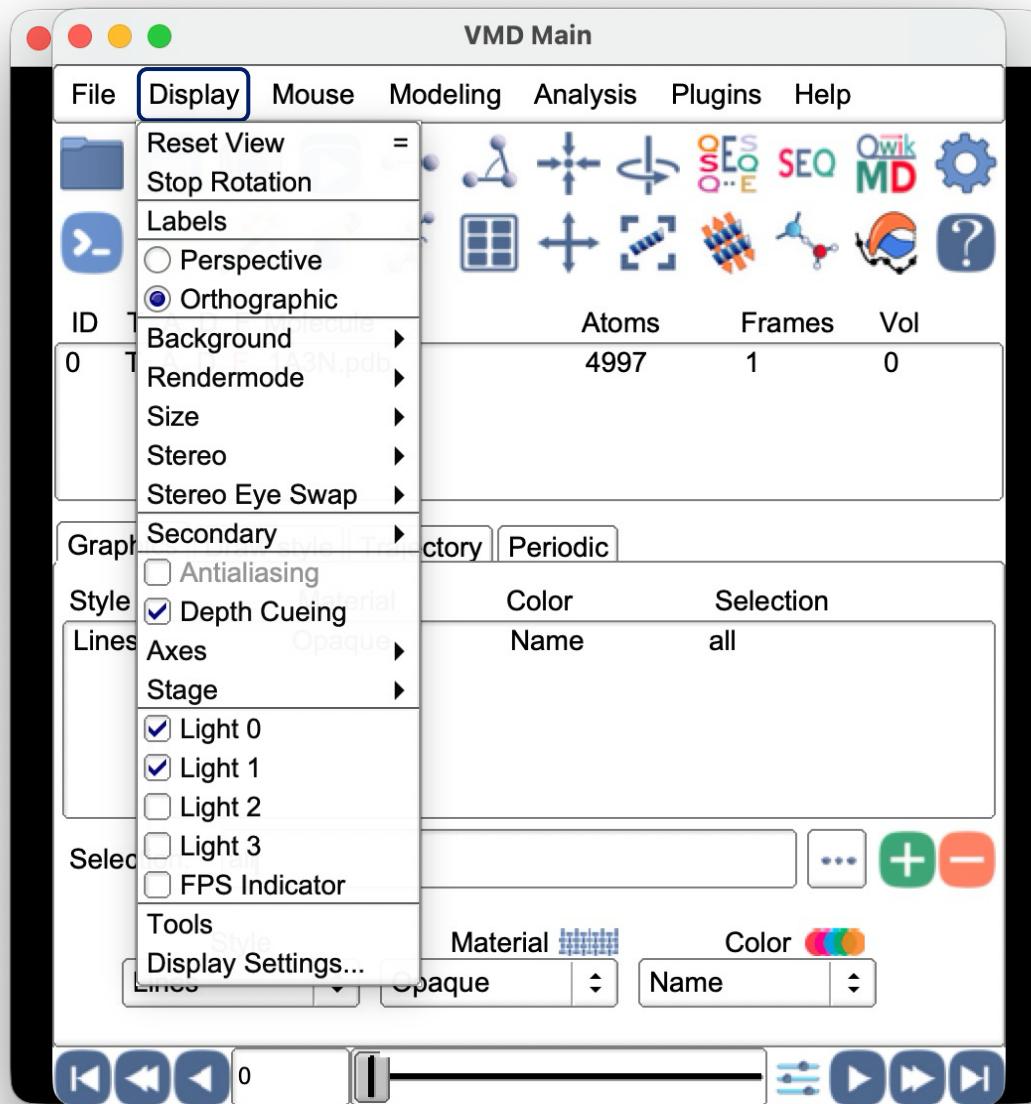
Selection: all

Style Material Color

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

Navigation: Back, Forward, Home, Zoom, Play, Stop, Next, Previous

Changing Display options



We can change under **Display**:

Perspective > Orthographic

Axes > Off

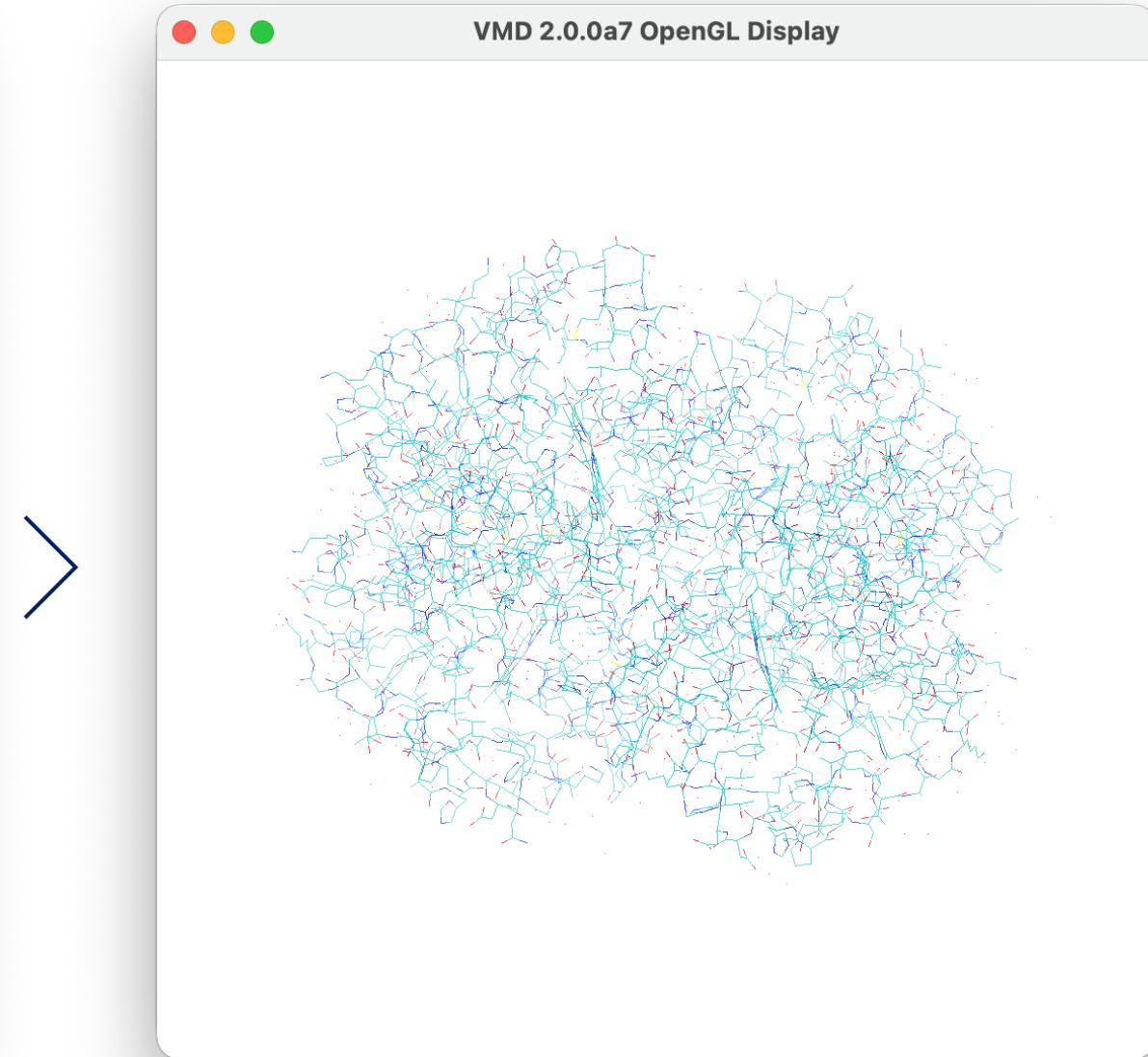
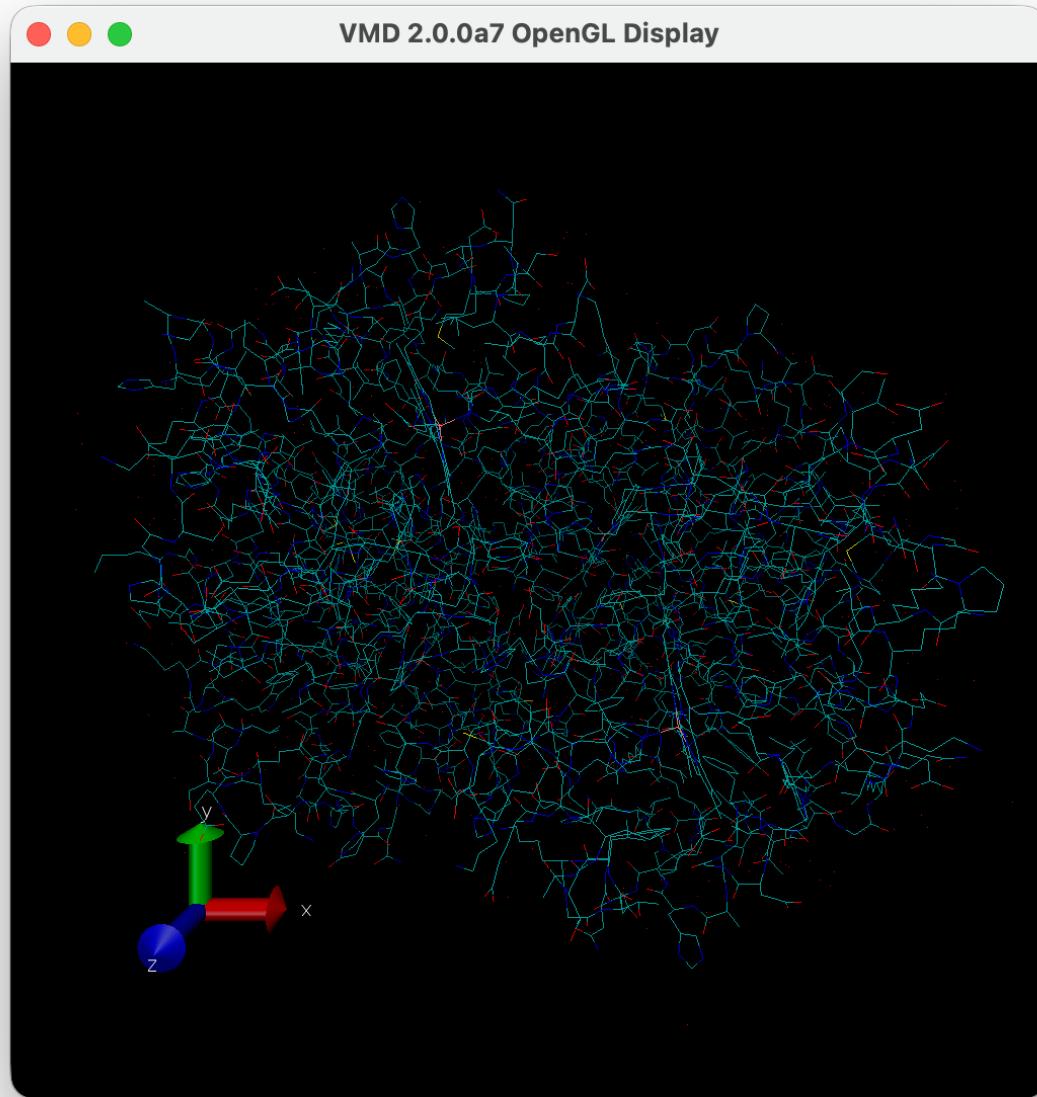
Background > White



In version 1.9.4

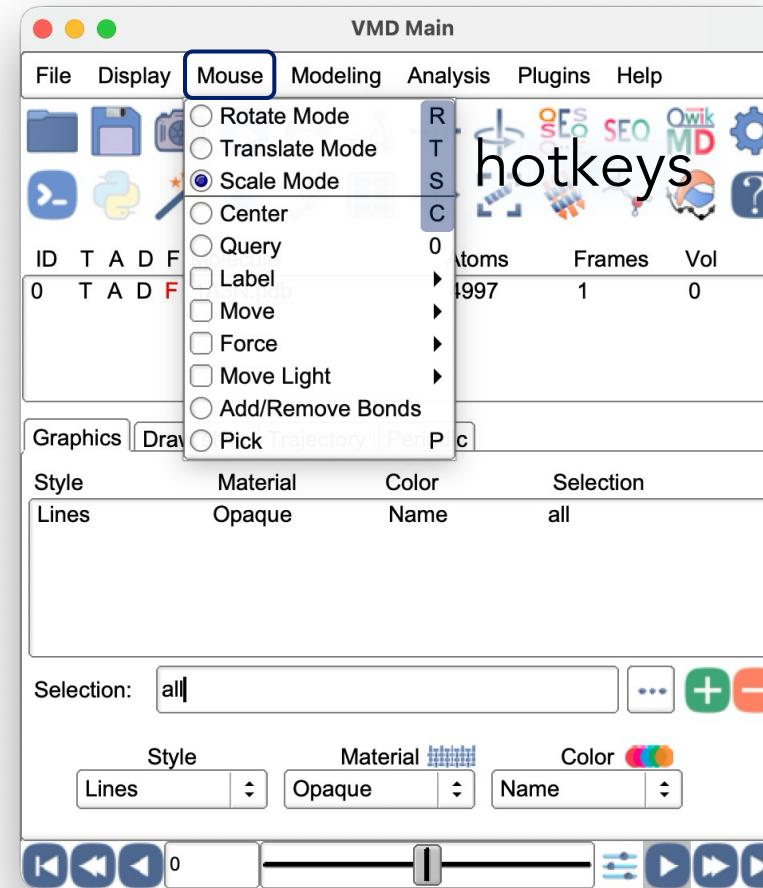
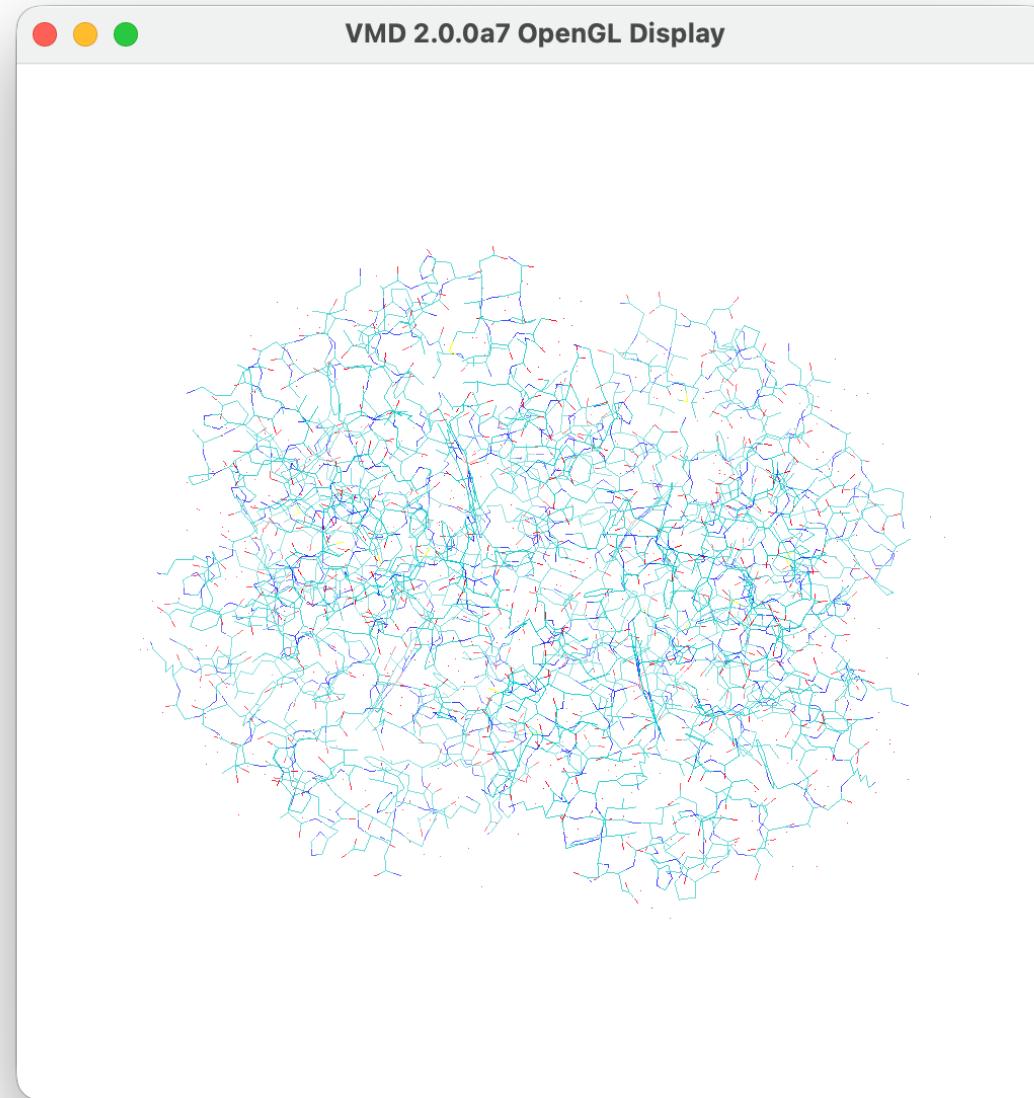
Graphics > Colors > Display > Background

Changing Display options

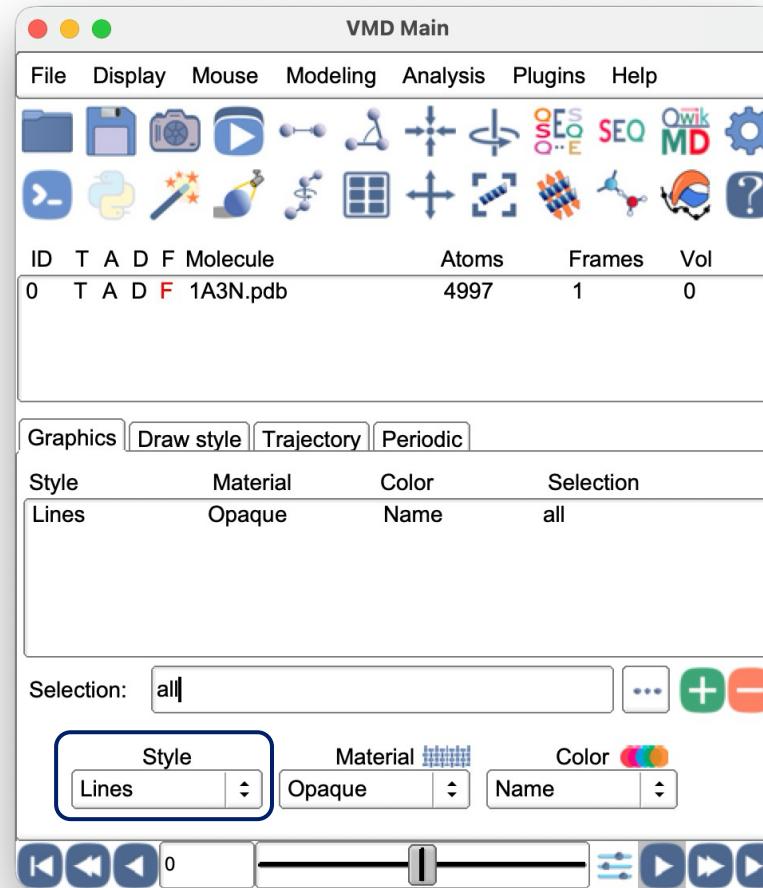
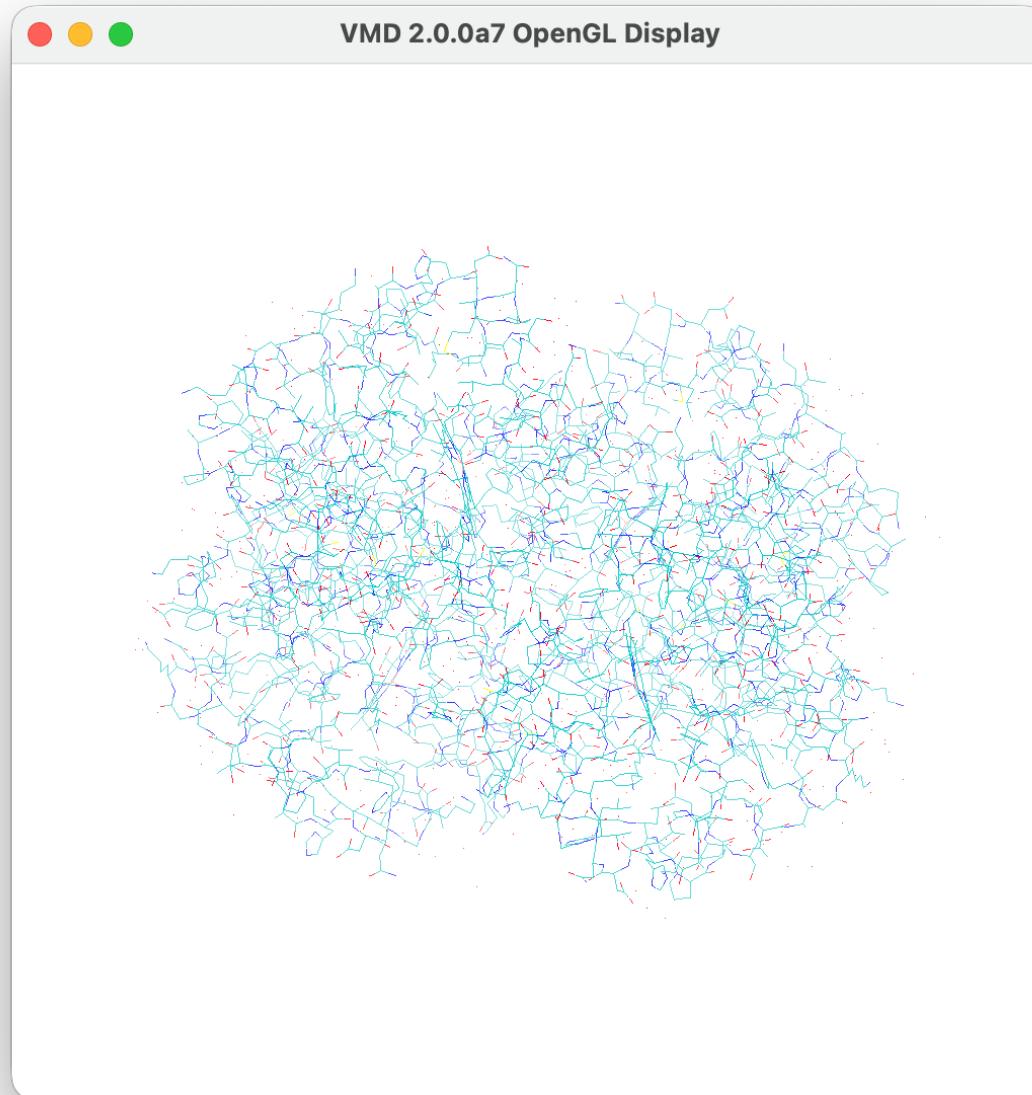


version 2.0.0

Exploring mouse actions

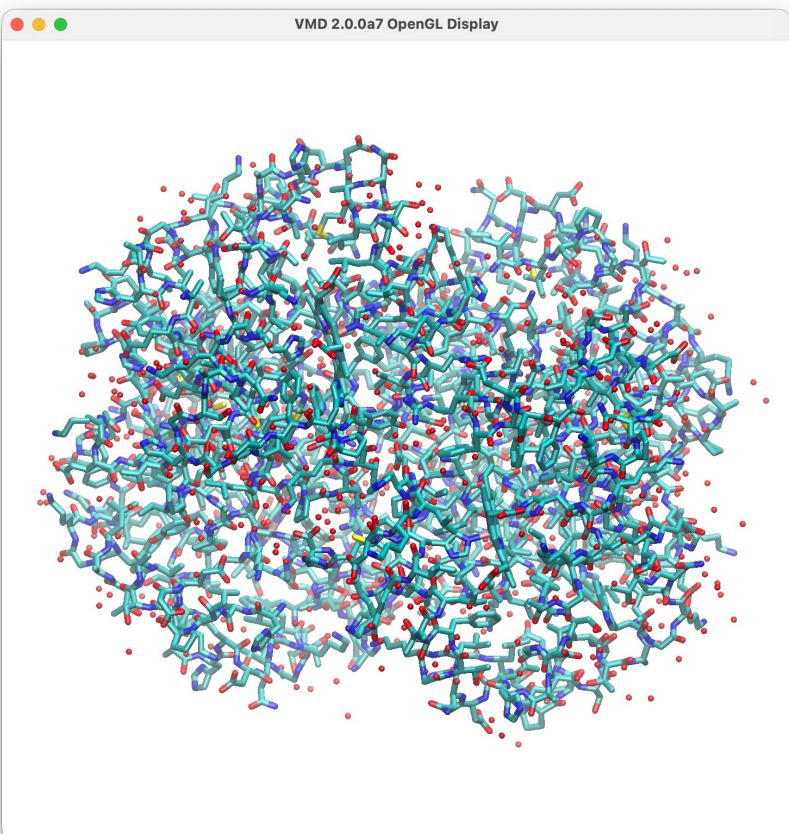


Changing the representation style

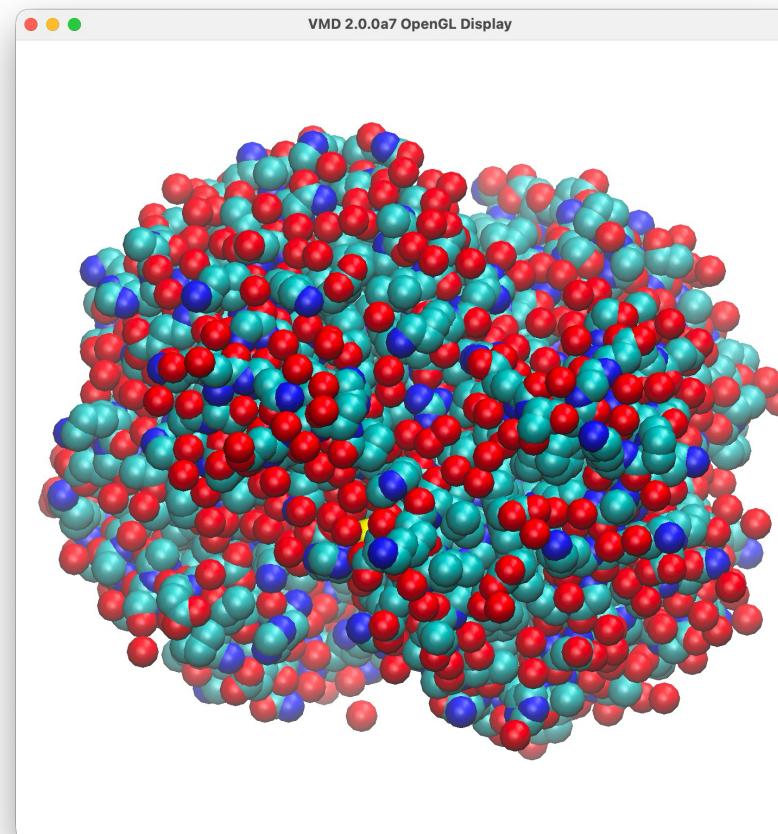


Changing the representation style

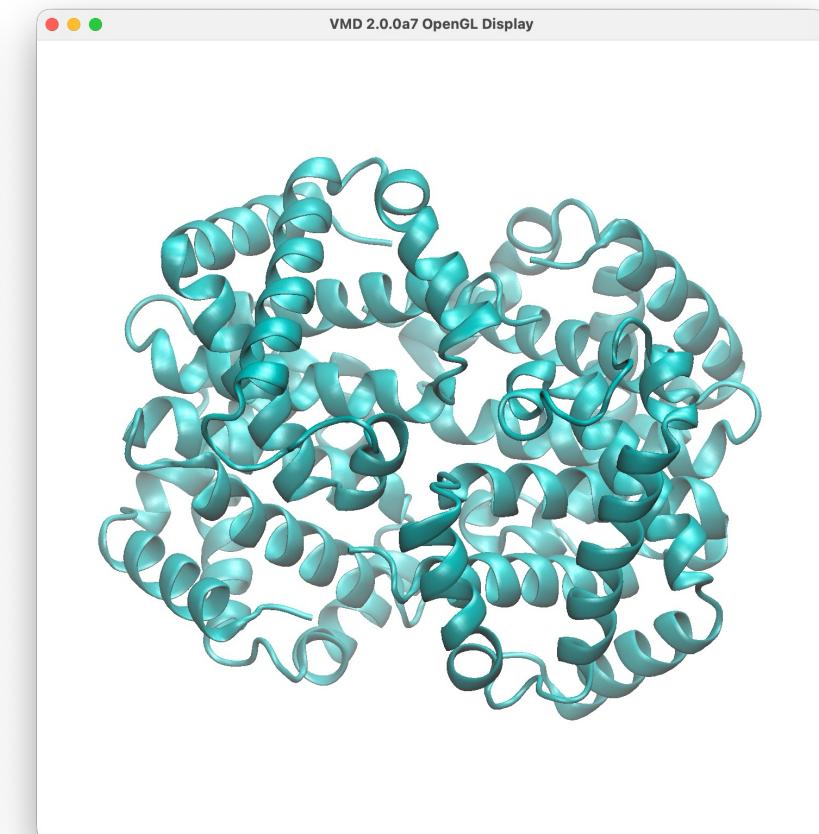
Licorice



VDW



NewCartoon



Style
Lines

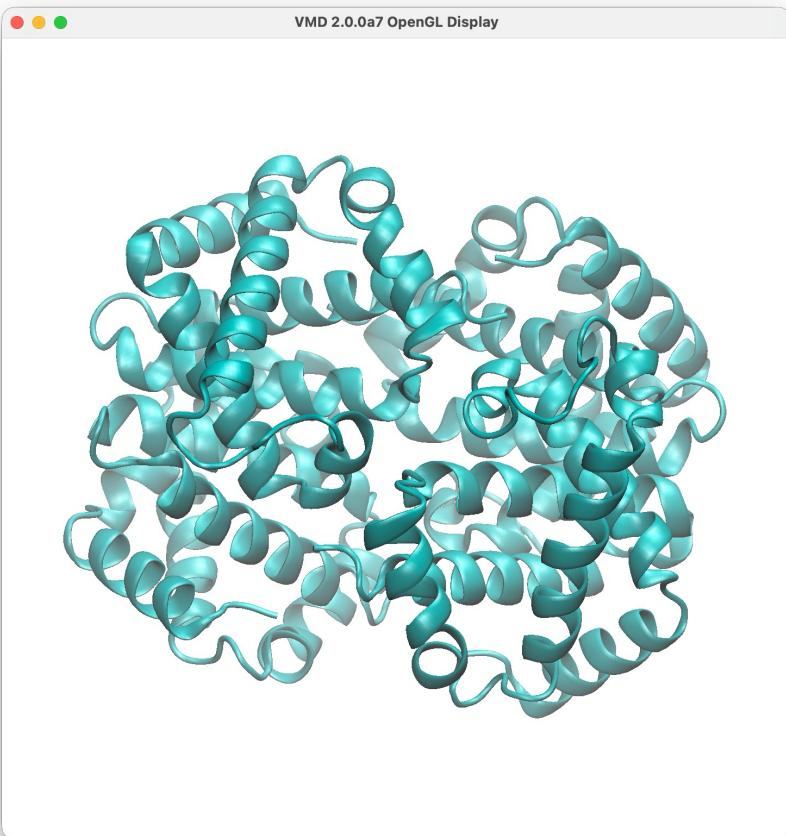
Material
Opaque

Color
Name

version 2.0.0

Changing the representation material

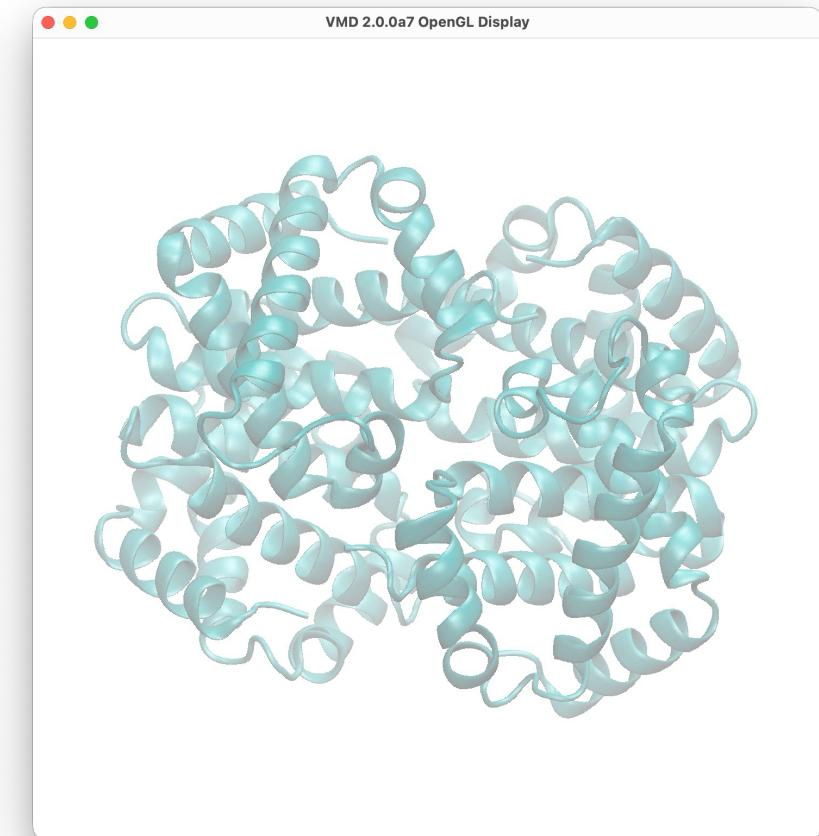
Opaque



A0Chalky



Transparent



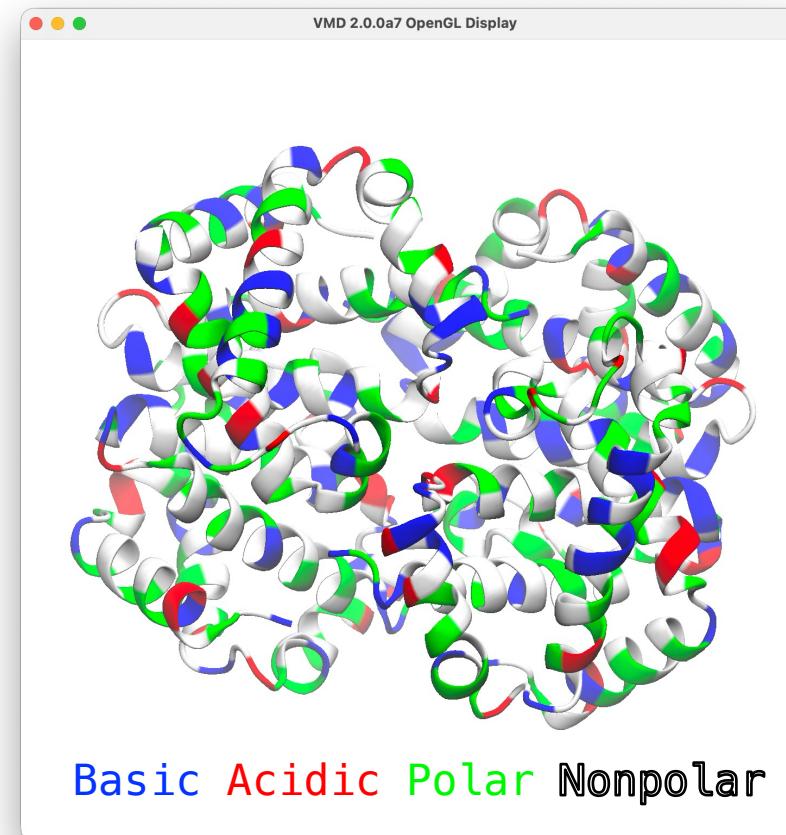
version 2.0.0

Changing the representation colors

ColorID (31)



ResType



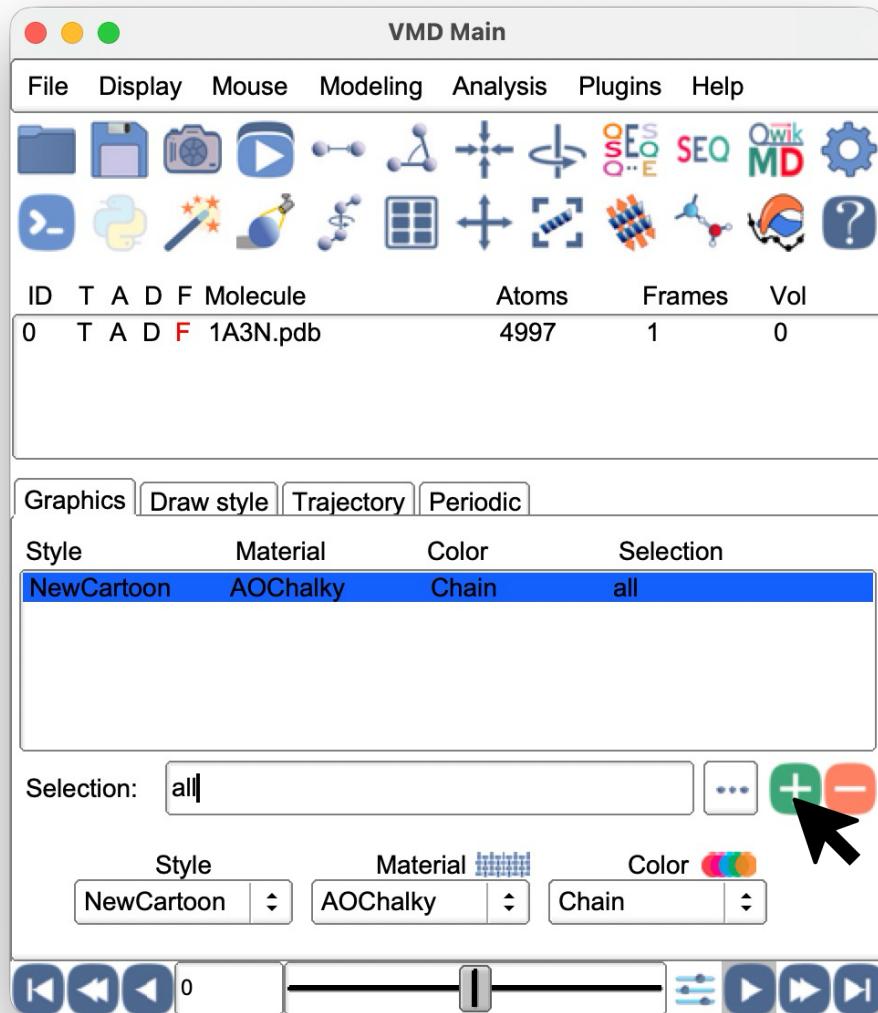
Chain



Style Material Color Name

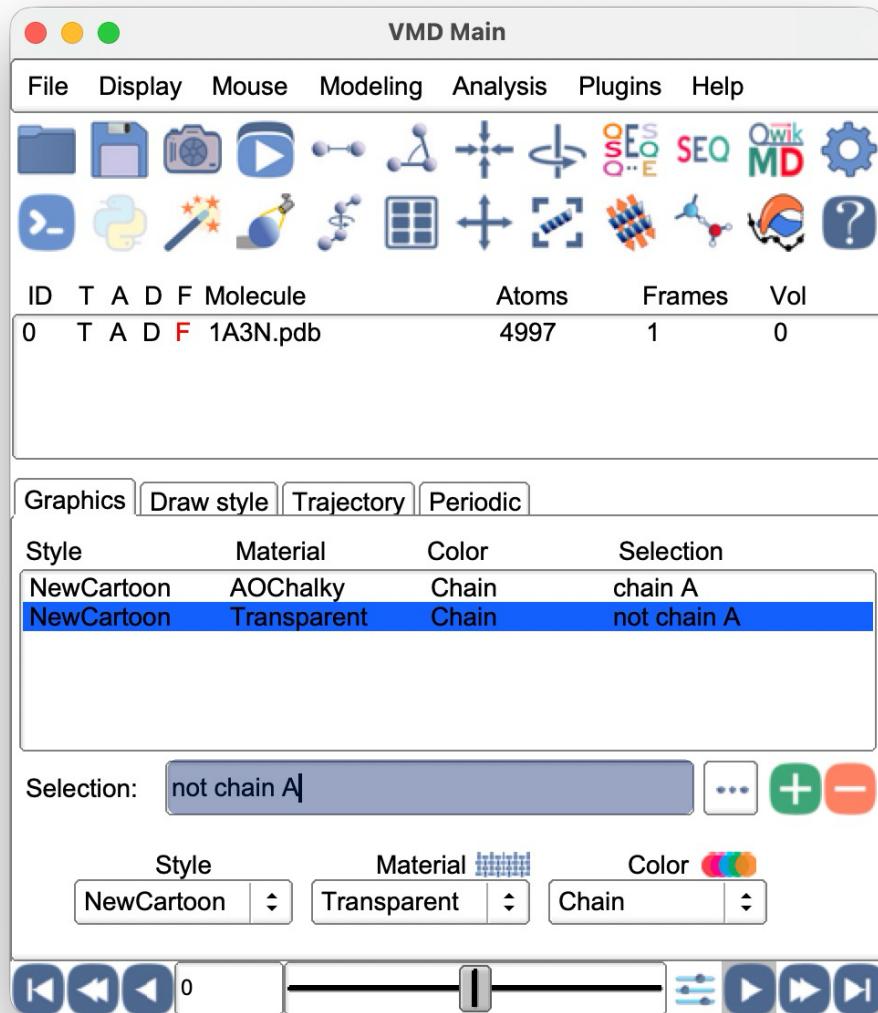
version 2.0.0

Adding different representations and selections

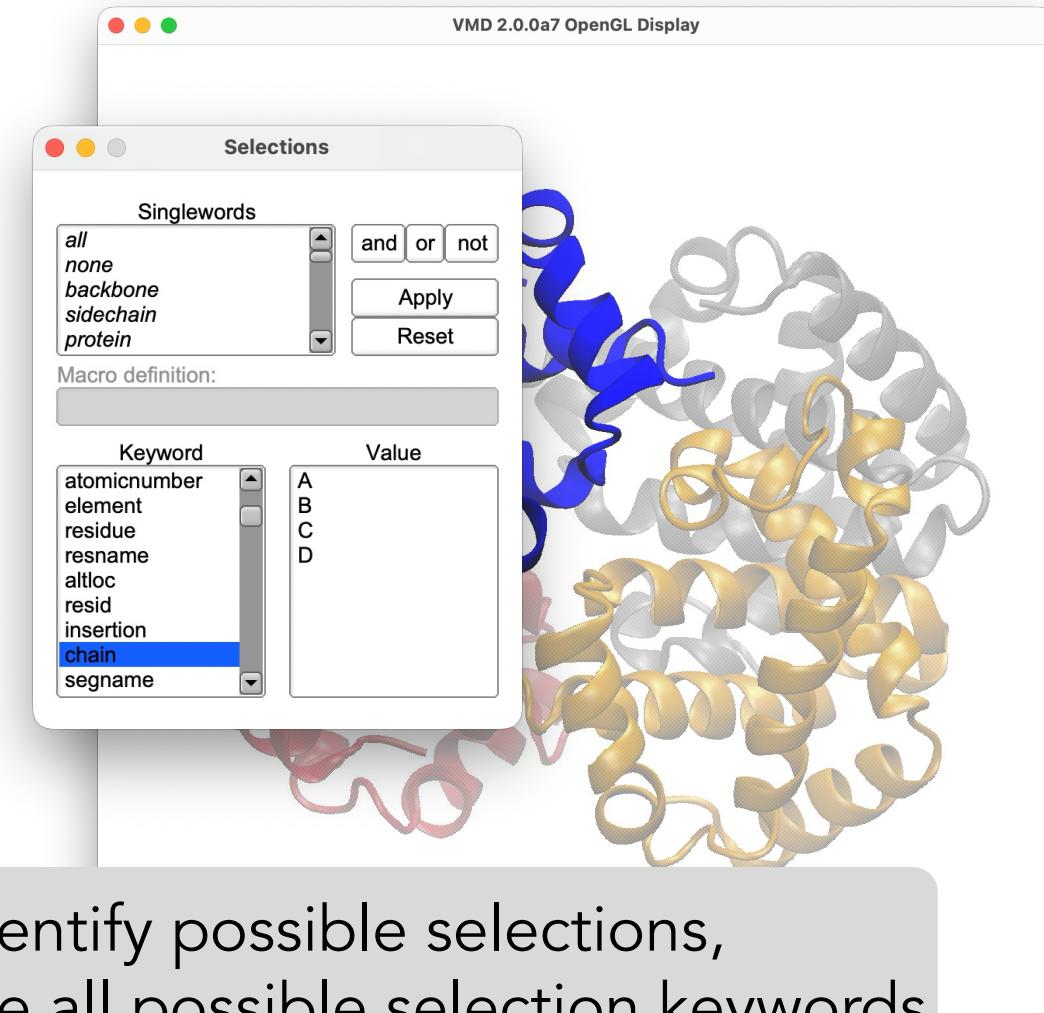
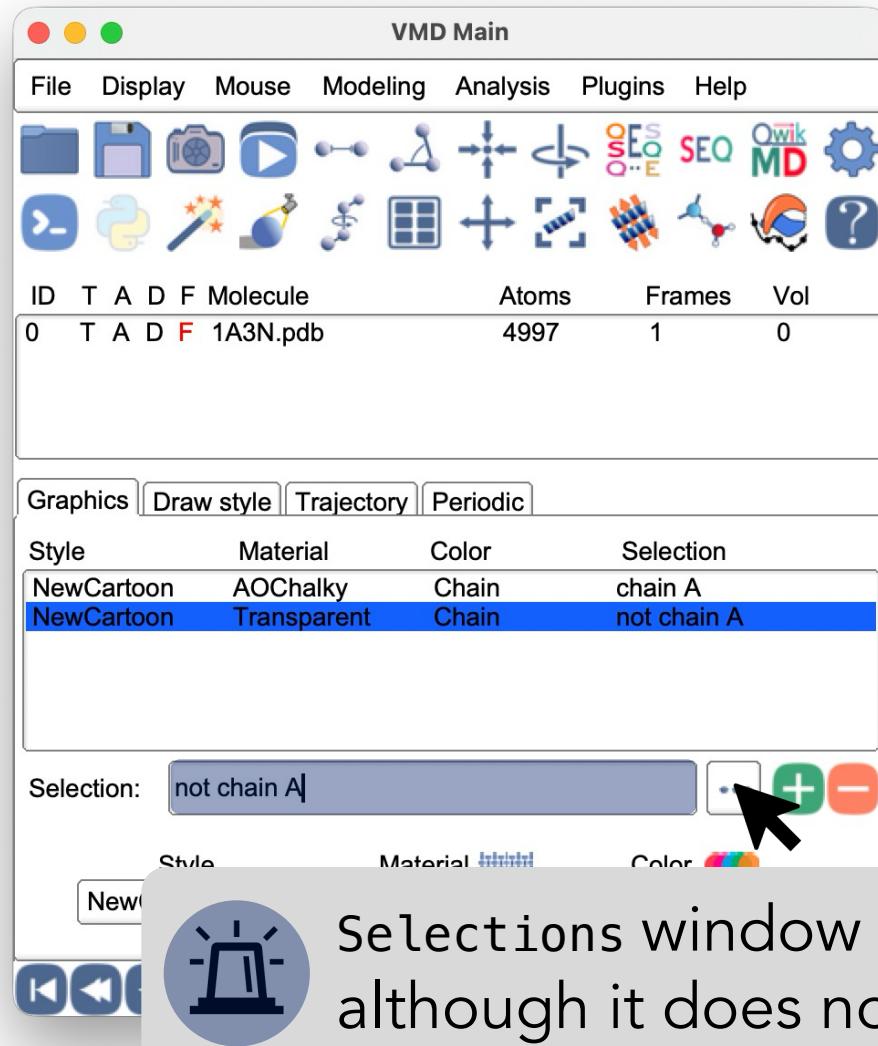


version 2.0.0

Adding different representations and selections



Adding different representations and selections

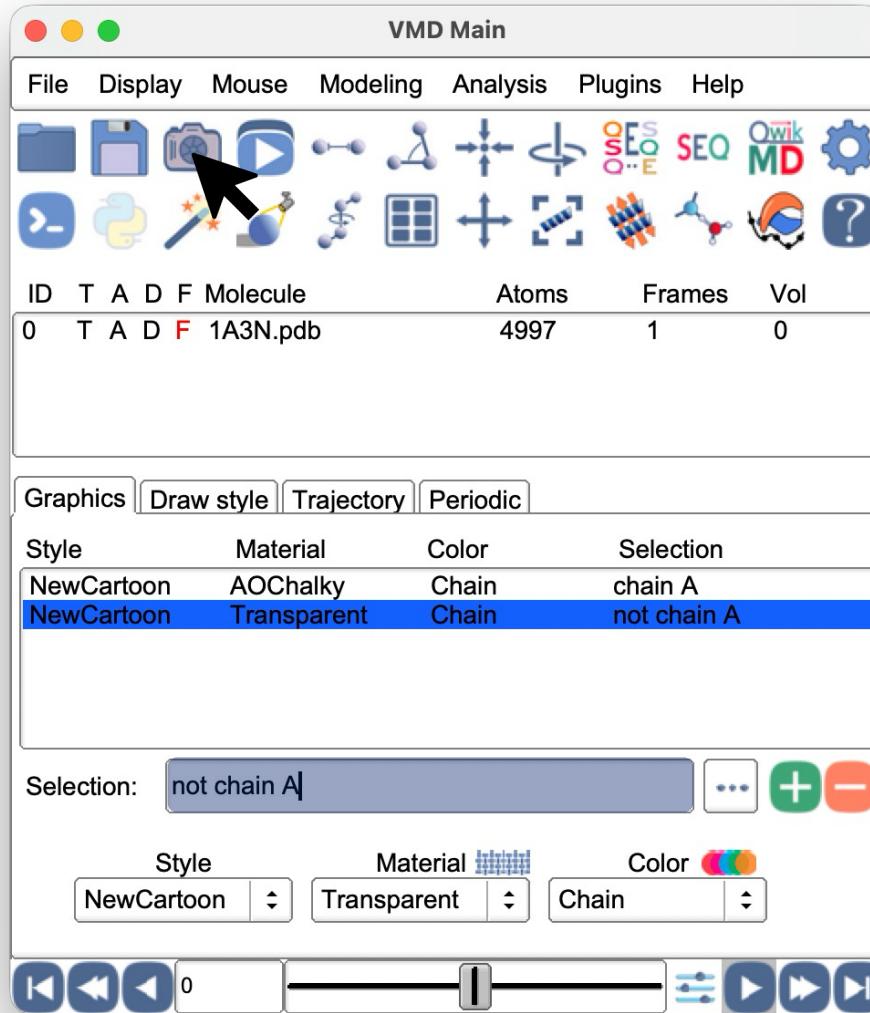


Selections window helps identify possible selections,
although it does not include all possible selection keywords

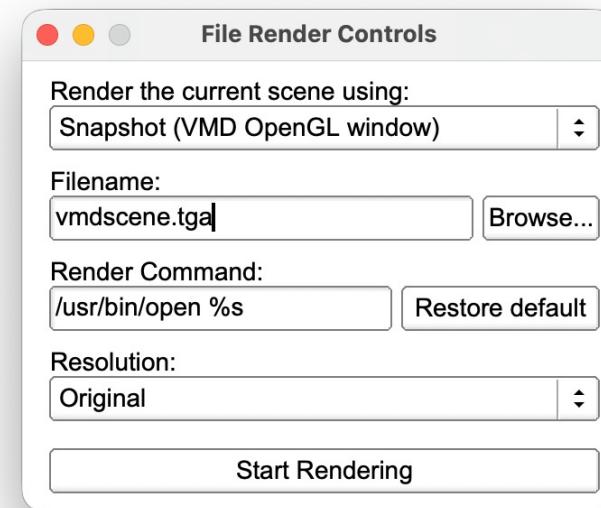
Examples: same ... as ..., within ... of ..., exwithin ... of ...

version 2.0.0

Rendering images



Alternatively: File > Render
(version 1.9.4)



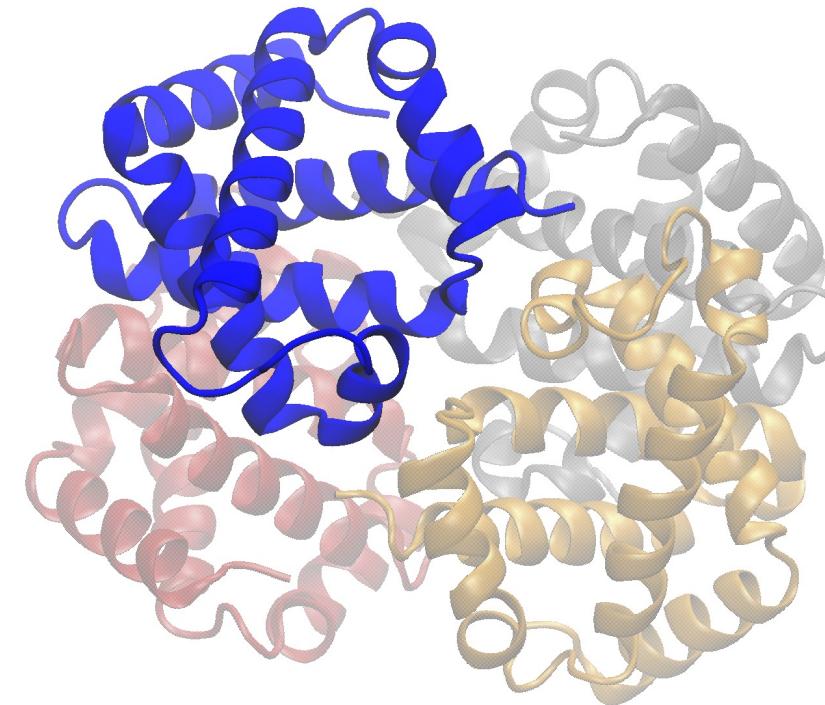
rendering engine
folder/file name

version 2.0.0

Rendering images



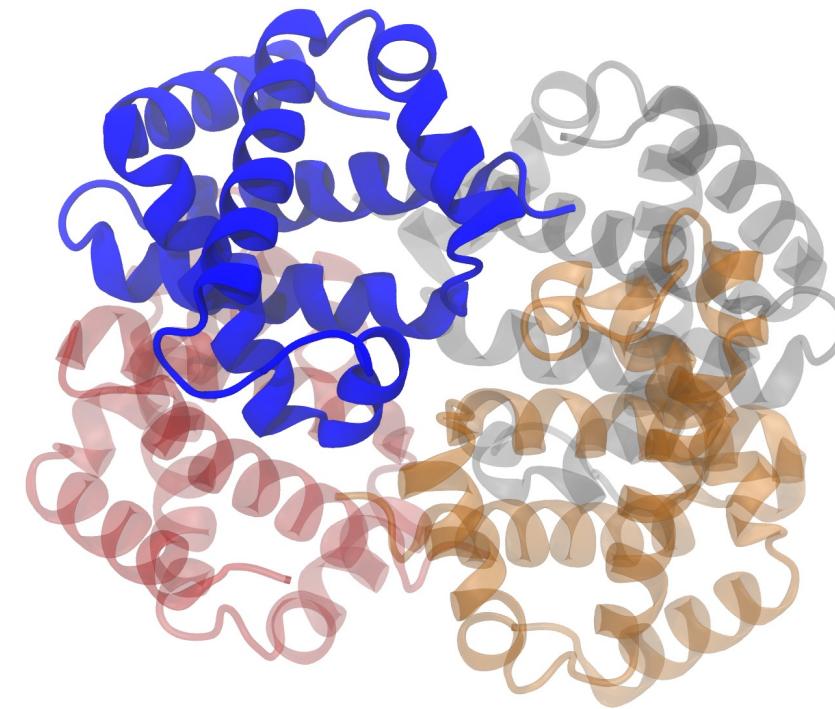
Snapshot



Rendering images

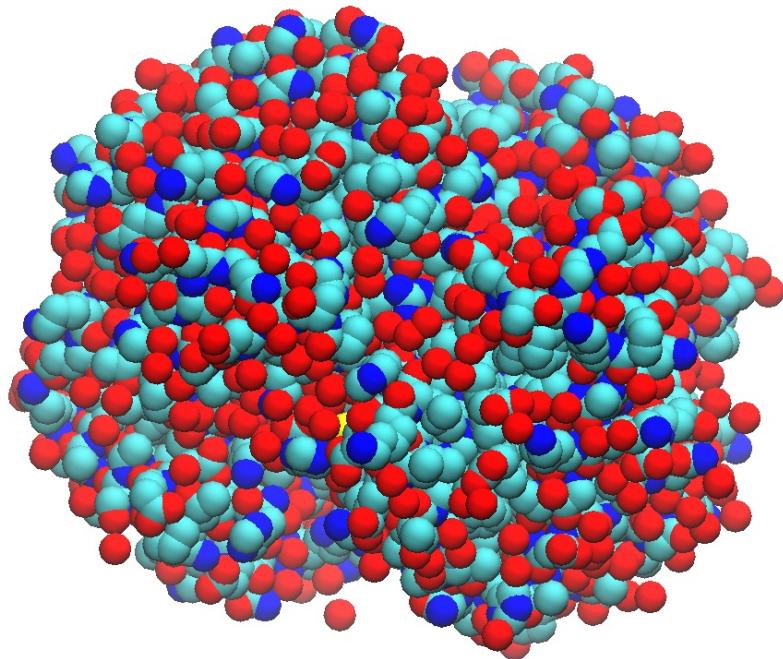


Tachyon Internal

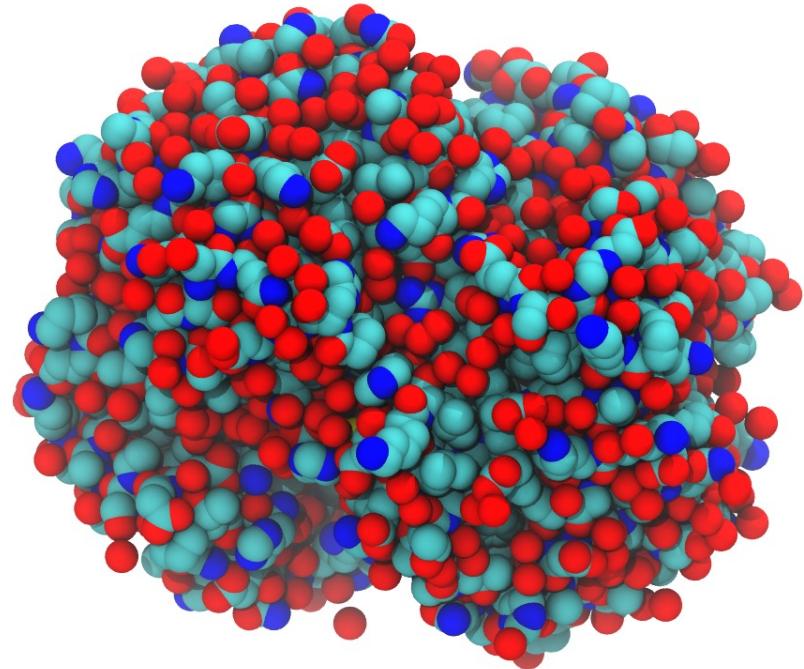


Rendering images

Snapshot



Tachyon Internal

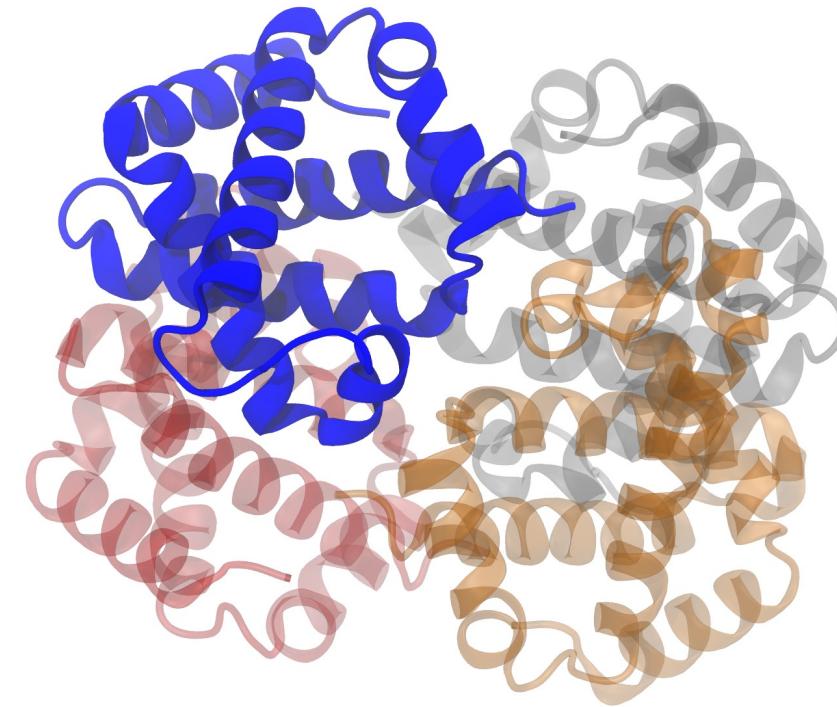


Shadows and depth cueing become
more apparent in Tachyon

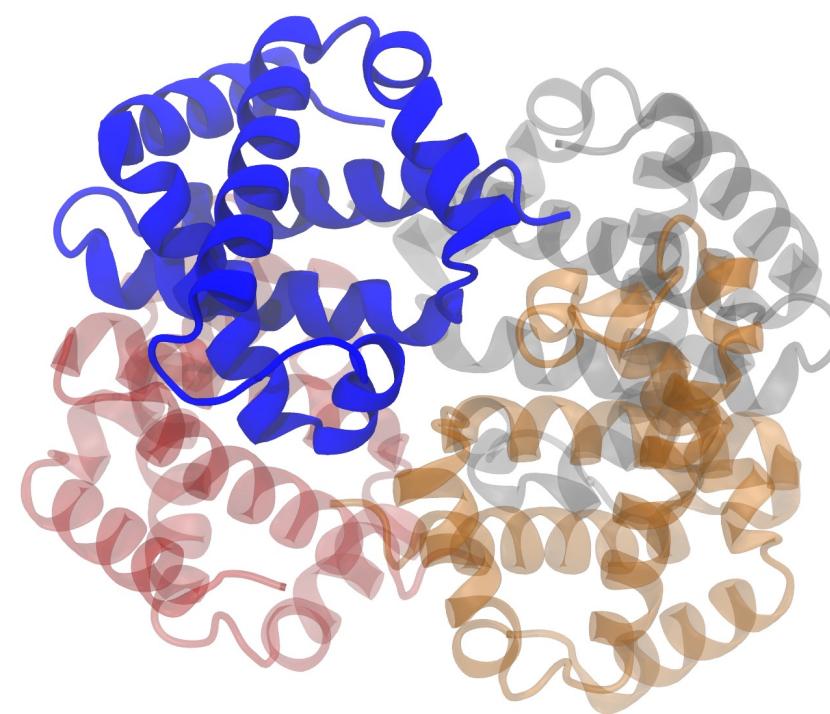
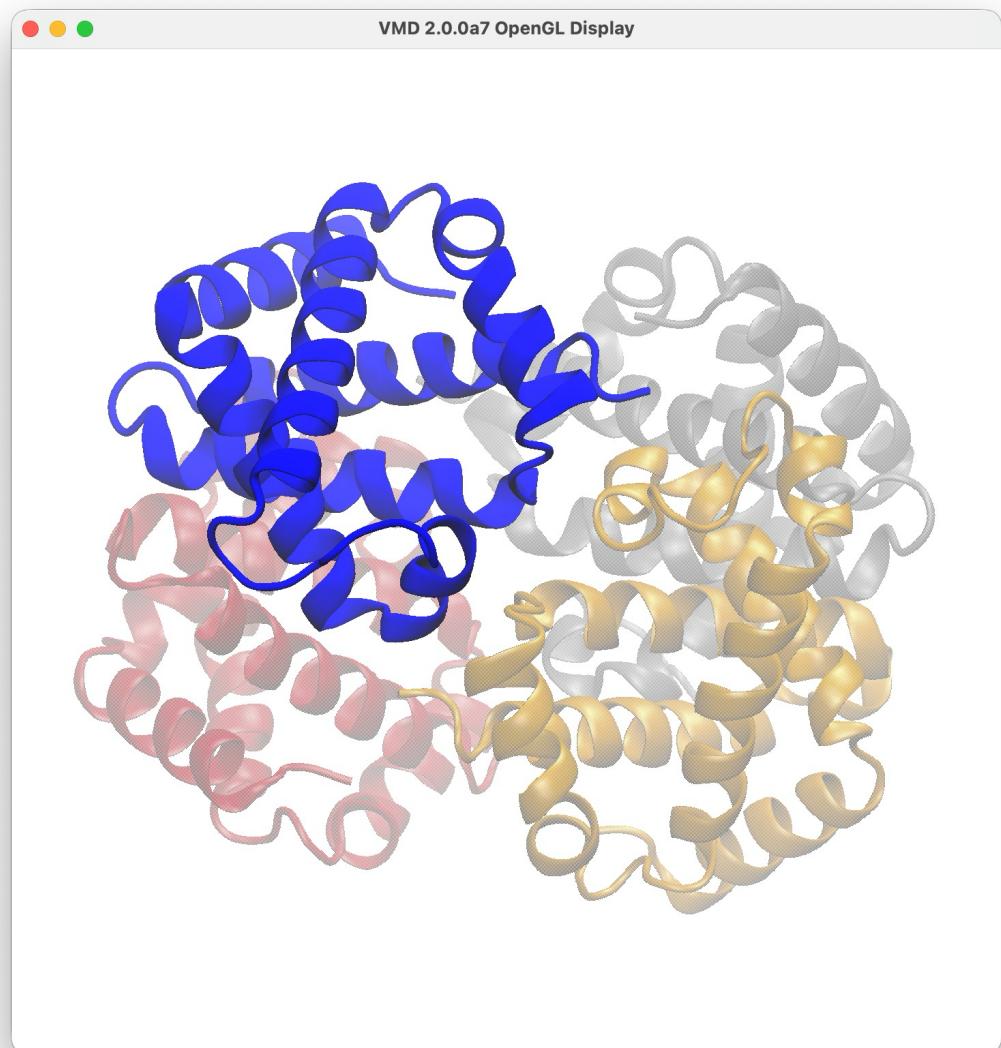
Rendering images



Tachyon Internal



Rendering images



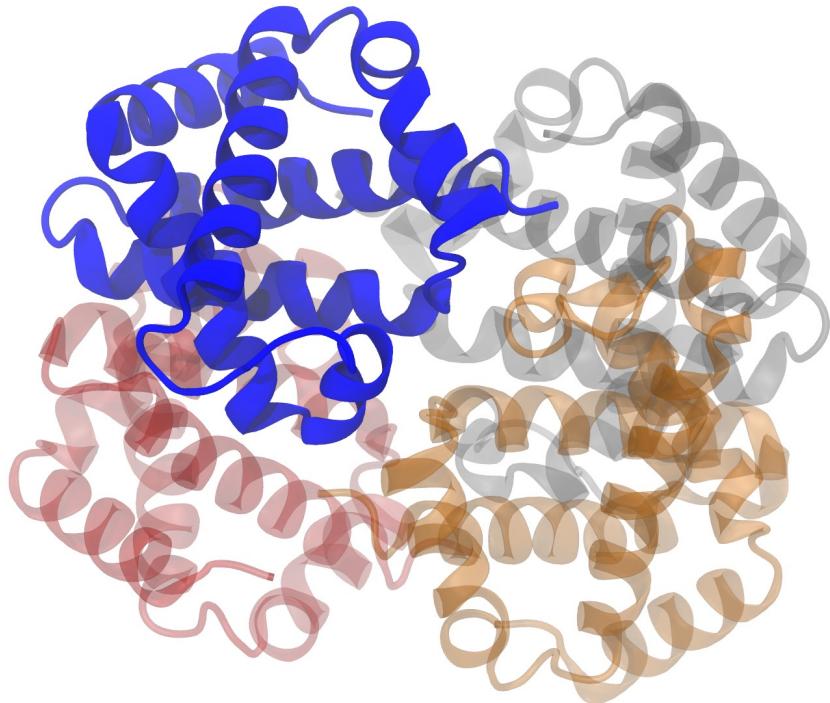
Tachyon



Note that a .dat file was generated

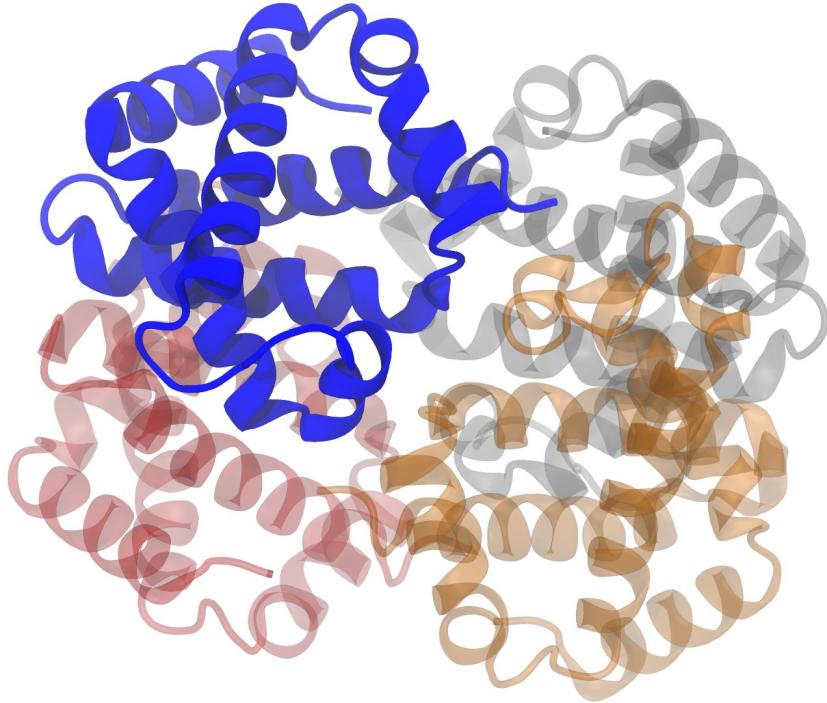
Rendering images

Tachyon Internal



vs.

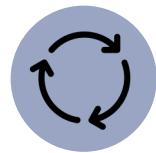
Tachyon



Tachyon (with the .dat file) allows for more control over resolution, lighting, performance, batching, even materials and colors

Rendering images

In search of the perfect figure
for publishing



Test different configurations and
settings (again and again)

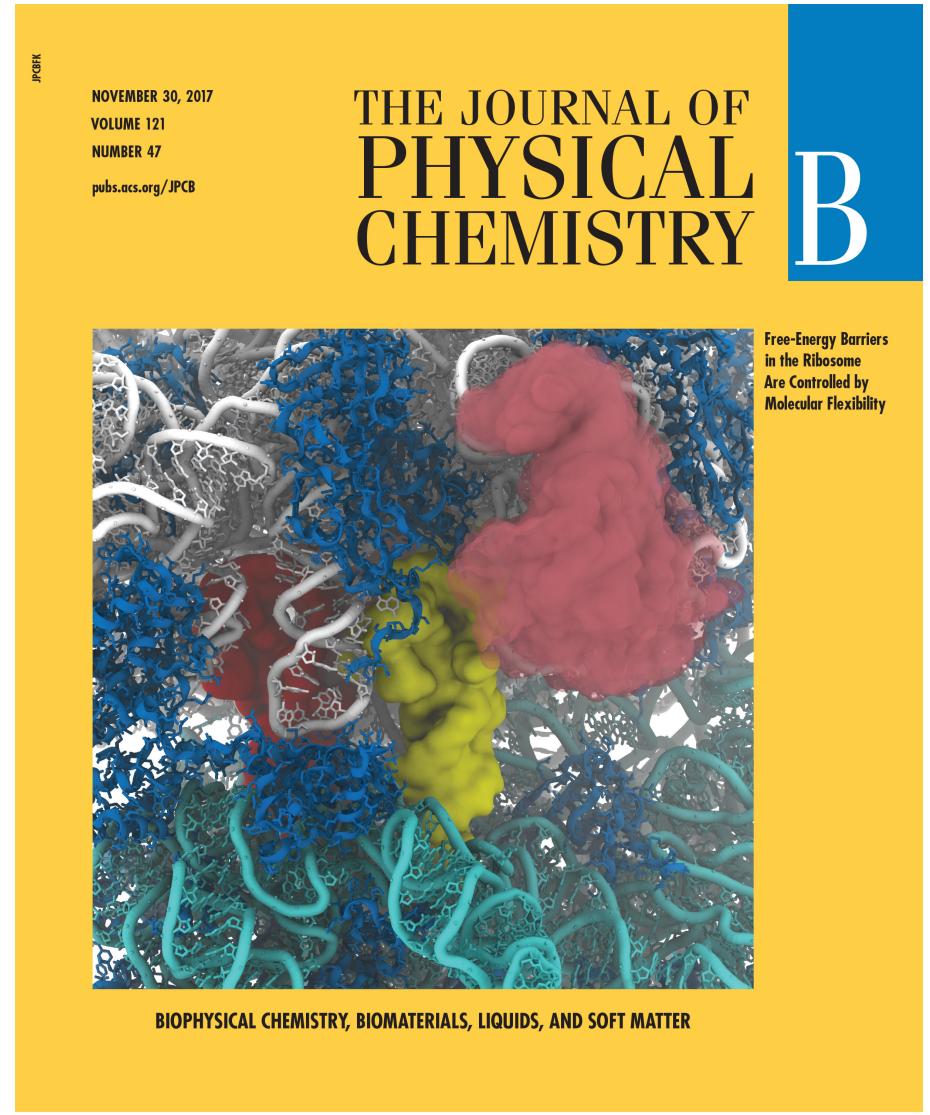


Consider using an inclusive color
scheme

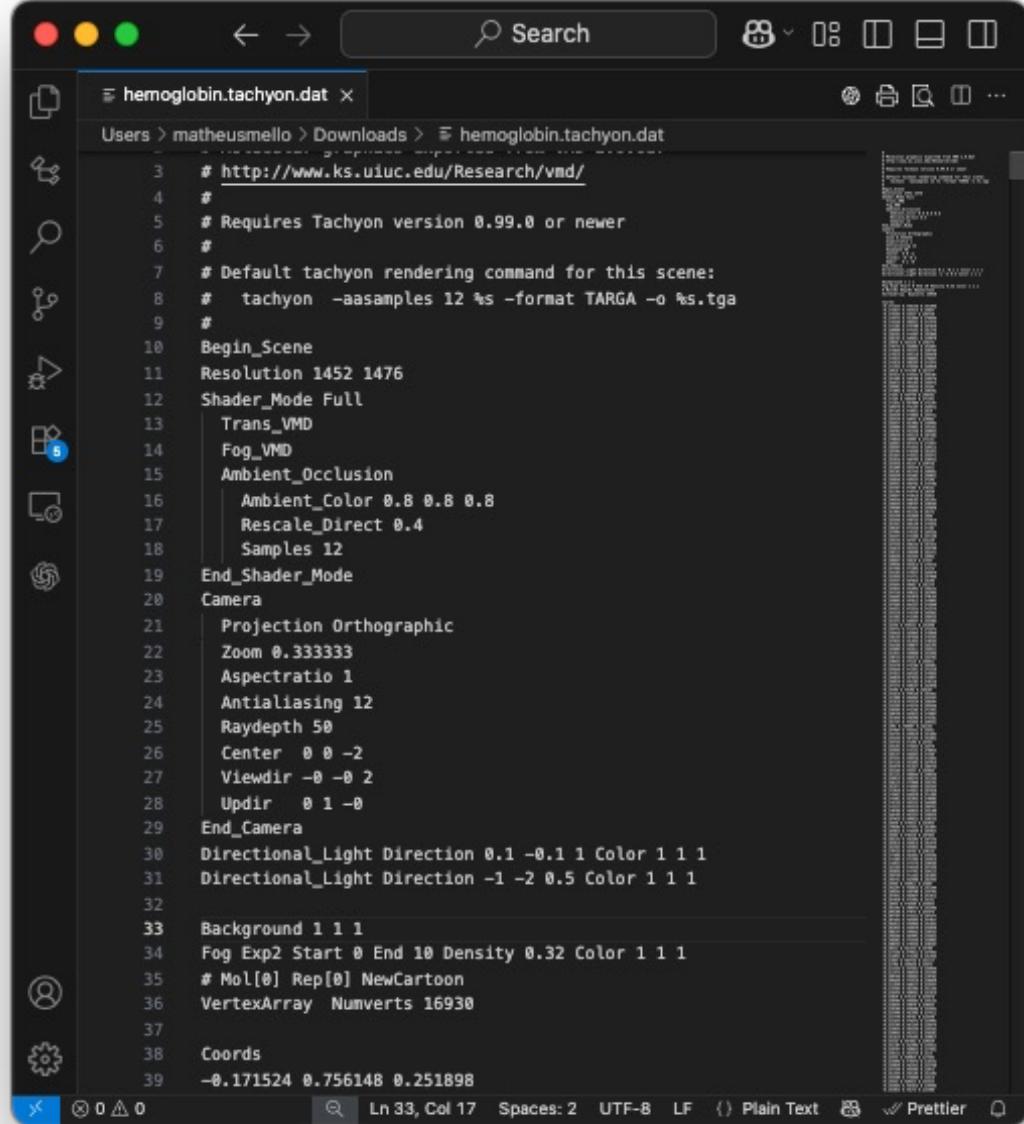


Save your progress (prevent
losing work and reproducibility)

~1000 versions of the figure with a
script changing material definitions



Rendering images



A screenshot of a terminal window titled 'hemoglobin.tachyon.dat'. The window shows a text-based configuration file for a rendering scene. The file includes settings for camera projection (Orthographic), lighting (Directional_Light), fog, and various rendering parameters like resolution and samples. 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
```

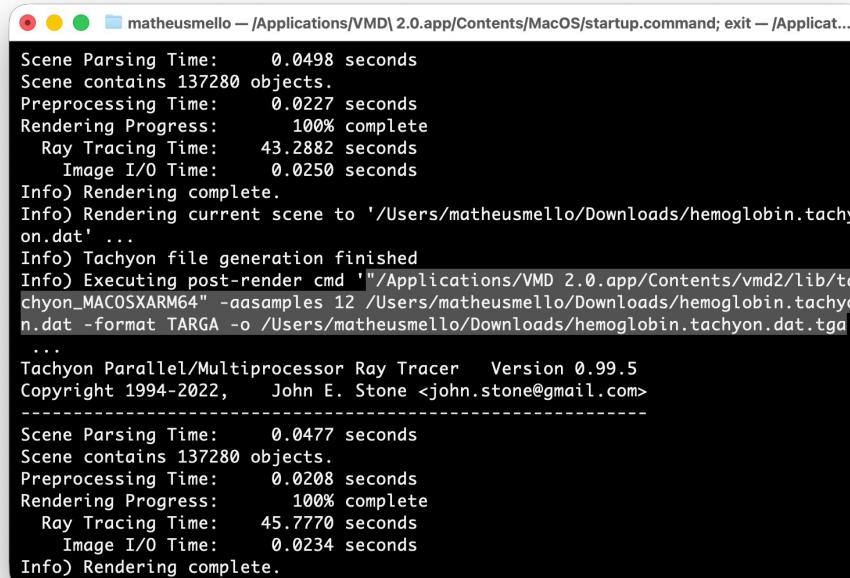
Ln 33, Col 17 Spaces: 2 UTF-8 LF Plain Text Prettier

.dat file: configures the scene

Some things we can change:

- Resolution > 2000 2000
- Fog | Density 0.32 > 0.20
- Colors, materials, lighting, etc.

VMD terminal



A screenshot of a 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 time taken for scene parsing, preprocessing, and rendering, along with the number of objects and the final rendered image file path. The terminal interface has a dark theme with light-colored text.

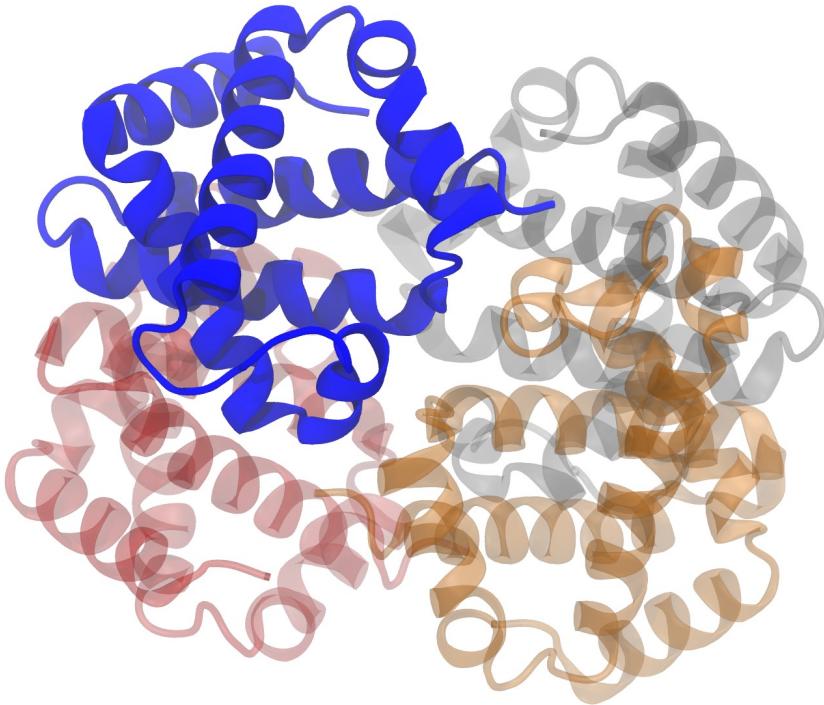
```
Scene Parsing Time: 0.0498 seconds
Scene contains 137280 objects.
Preprocessing Time: 0.0227 seconds
Rendering Progress: 100% complete
Ray Tracing Time: 43.2882 seconds
Image I/O Time: 0.0250 seconds
Info) Rendering complete.
Info) Rendering current scene to '/Users/matheusmello/Downloads/hemoglobin.tachyon.dat' ...
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

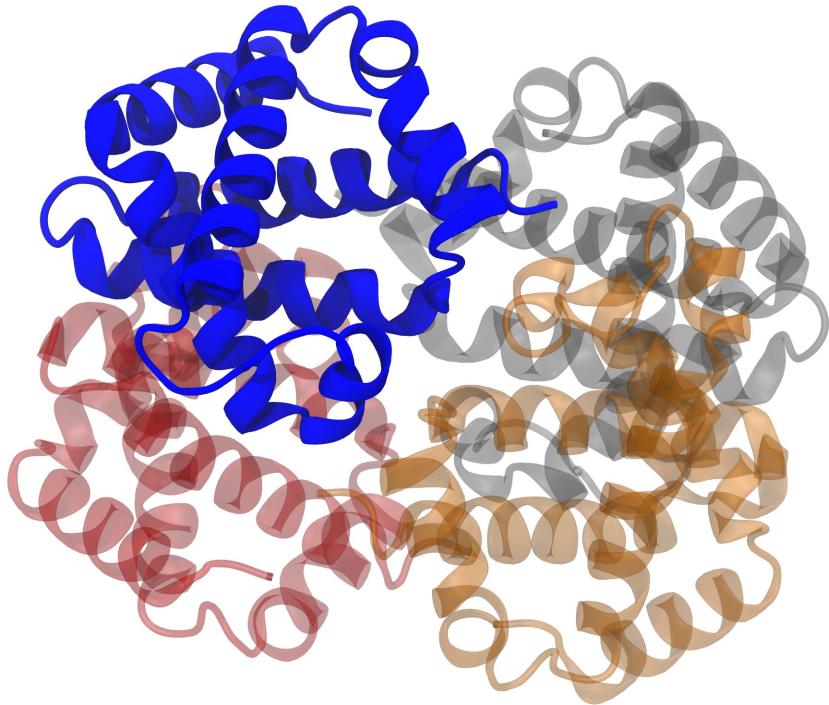
version 2.0.0

Rendering images

Tachyon



edited .dat file



On a new terminal, paste the rendering command

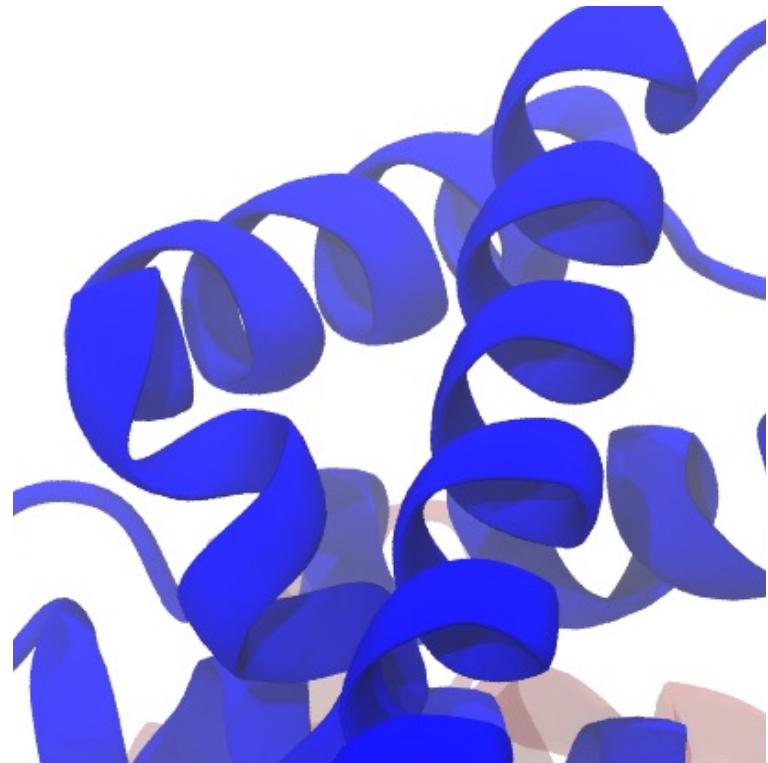
Tachyon's path
depends on your
installation

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

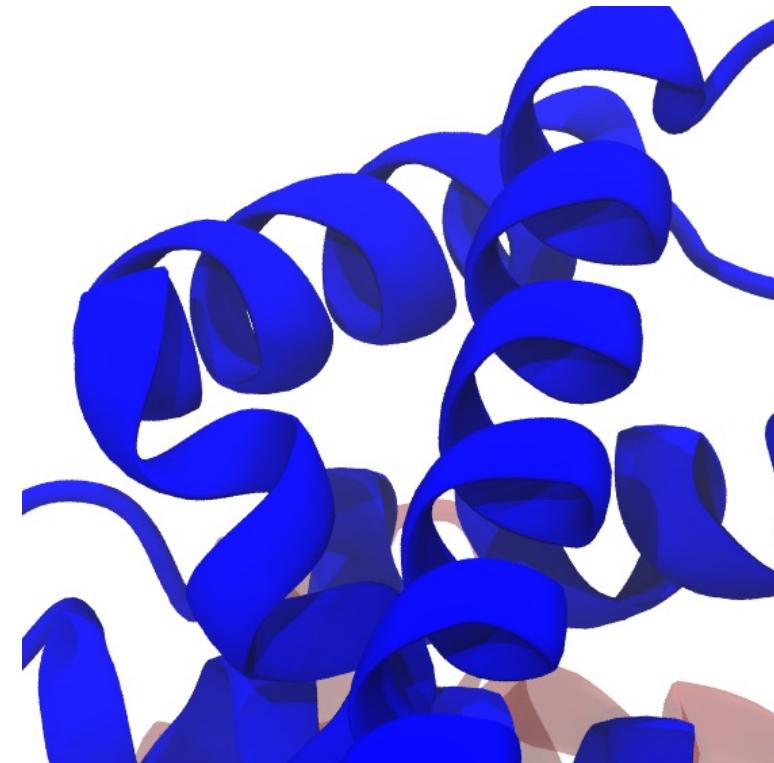
version 2.0.0

Rendering images

Tachyon



edited .dat file



On a new terminal, paste the rendering command

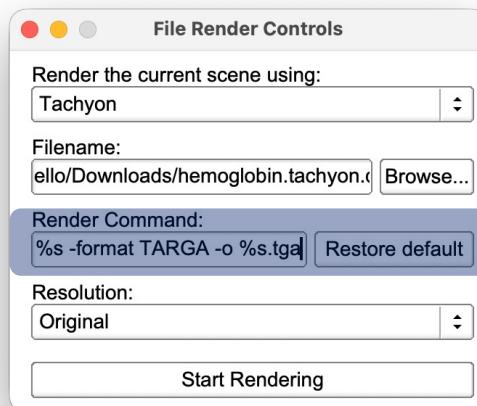
Tachyon's path
depends on your
installation

```
"/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:

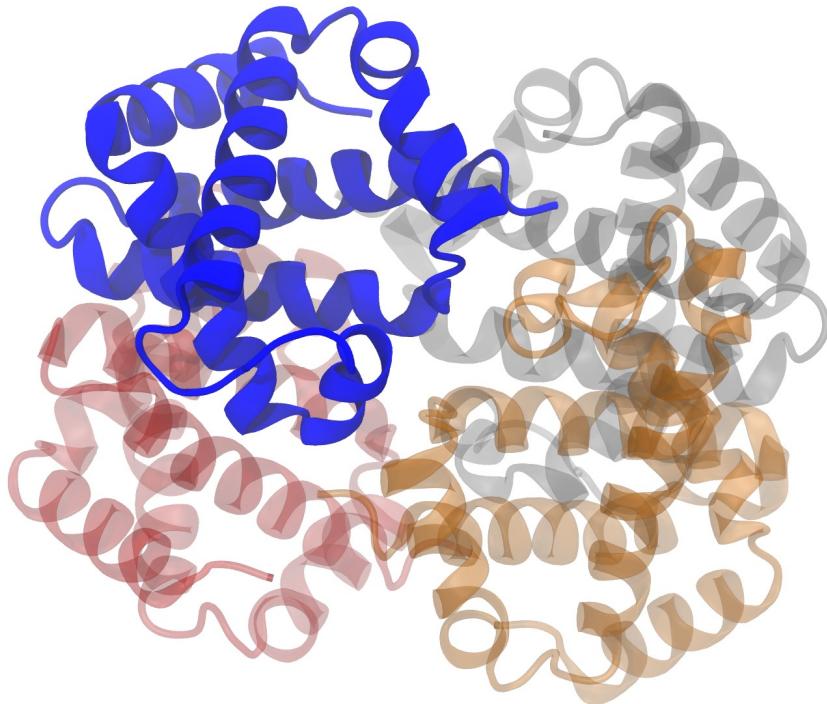
```
"/Applications/VMD 2.0.app/Contents/vmd2/lib/tachyon_MACOSXARM64" -  
aasamples 12 %s -fullshade -auto_skylight 1.4 -format TARGA -o %s.tga
```



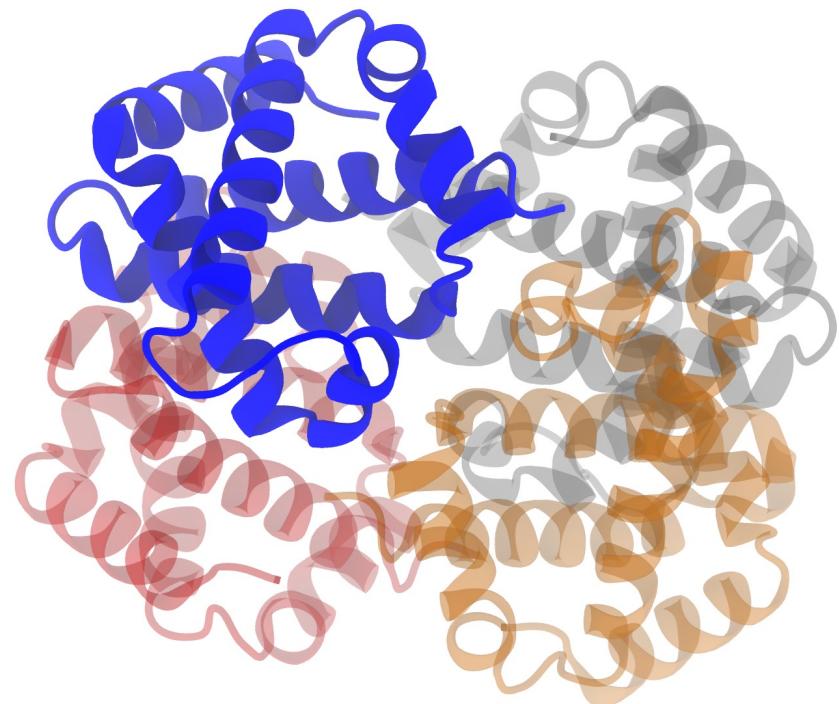
It will take considerably longer to render

Rendering images

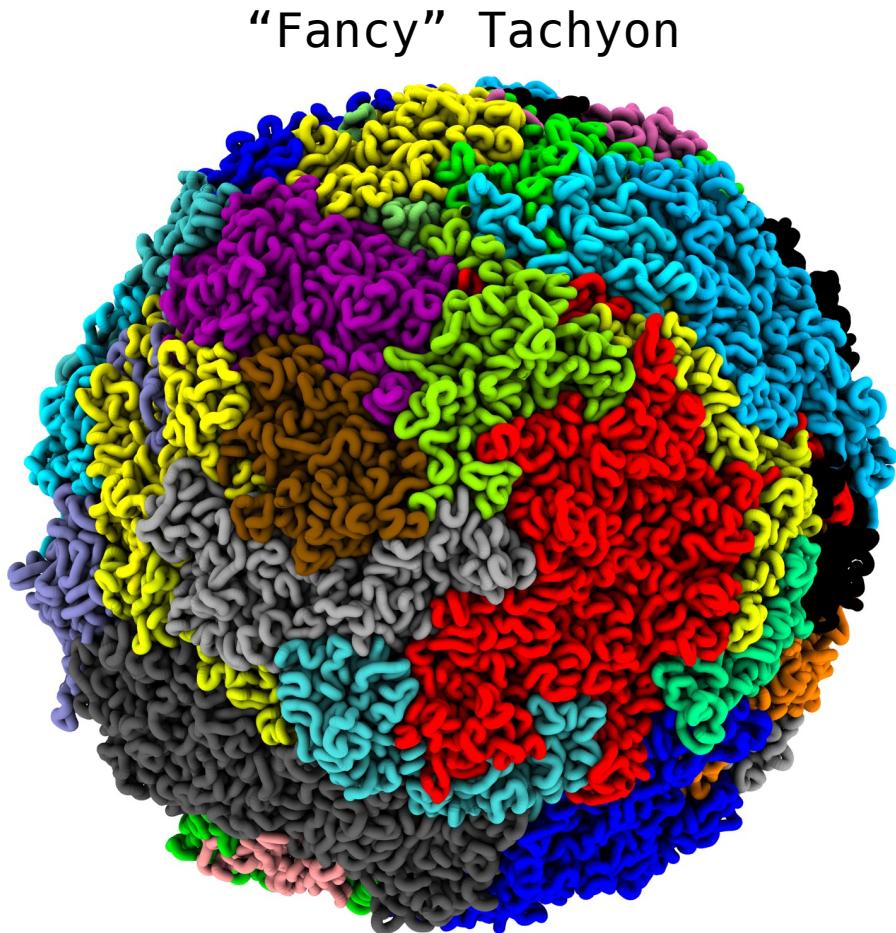
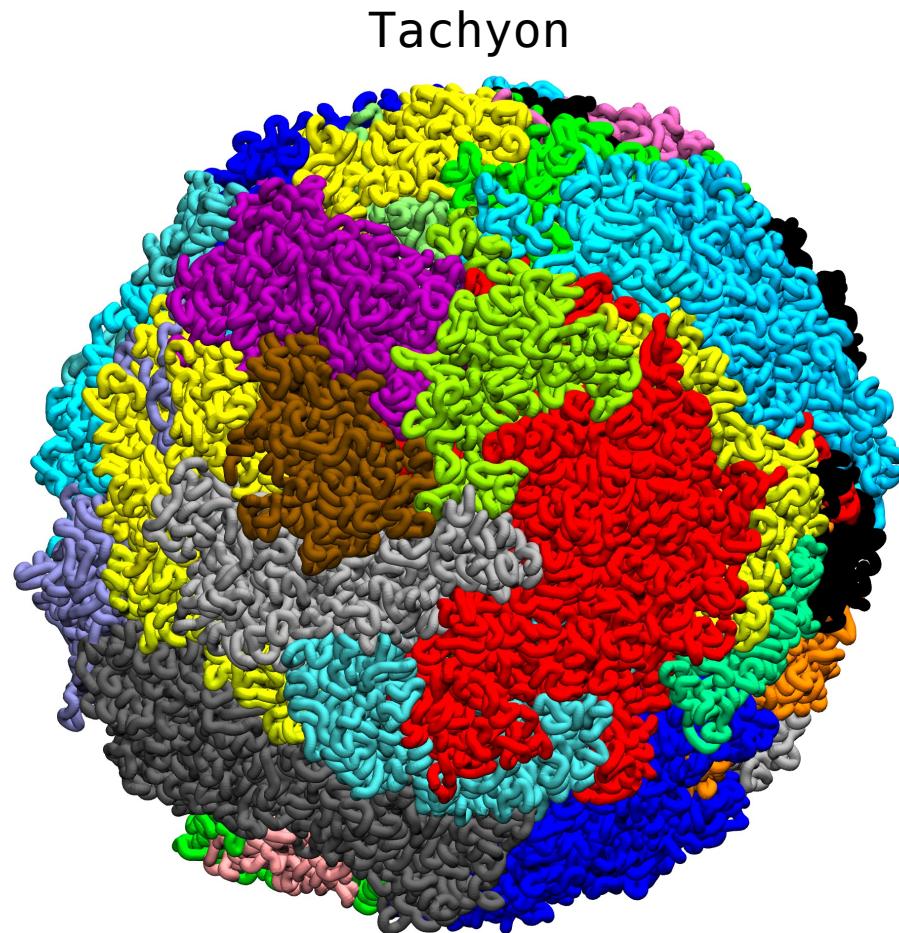
Tachyon



“Fancy” Tachyon

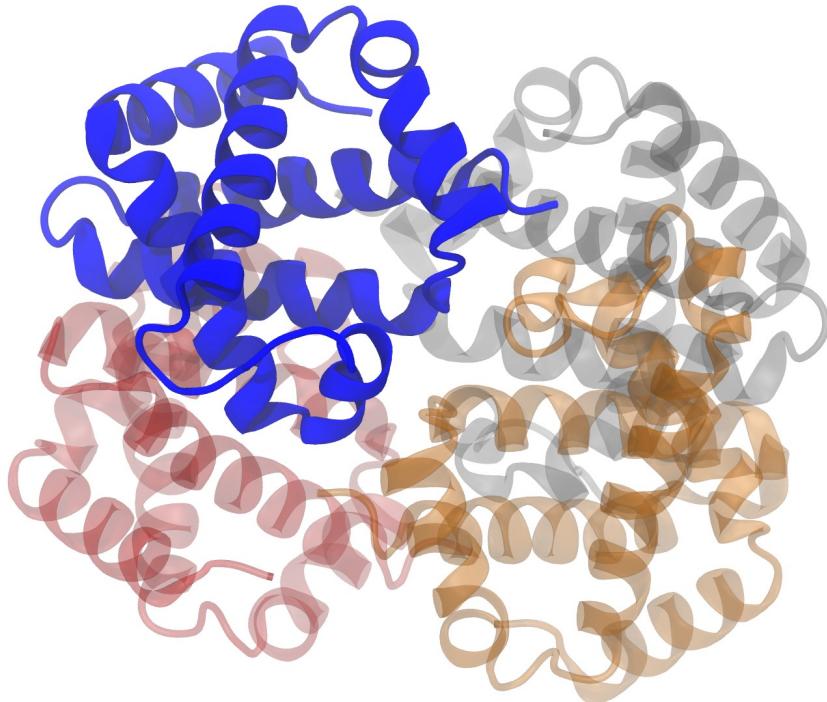


Rendering images

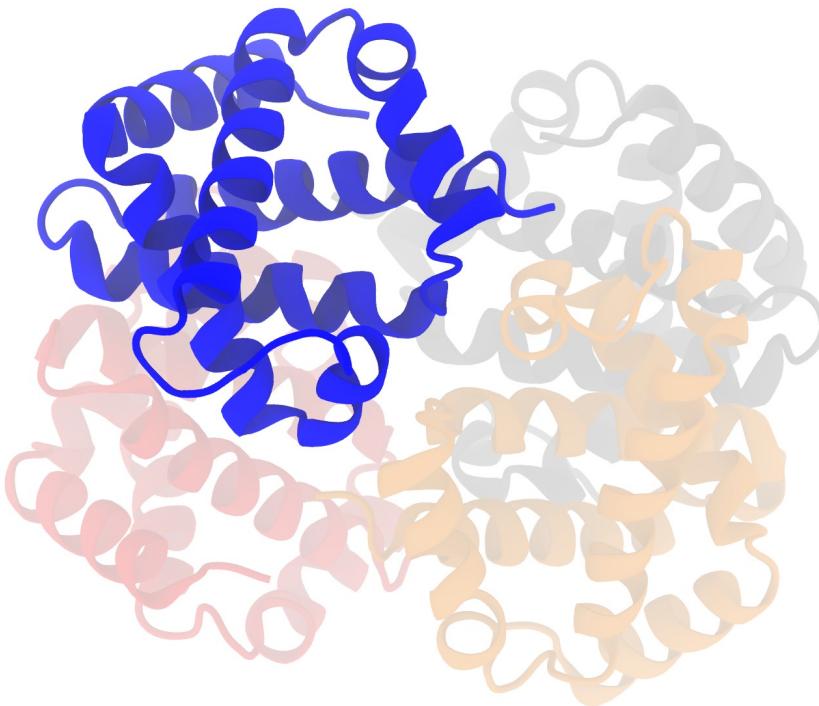


Rendering images

Tachyon

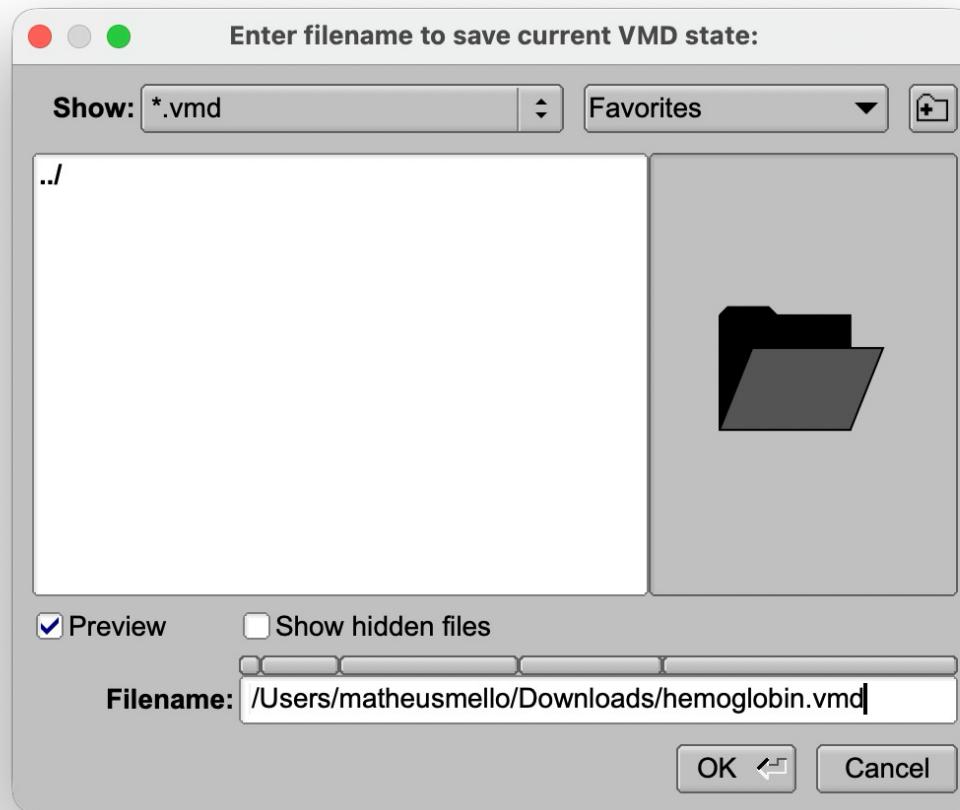
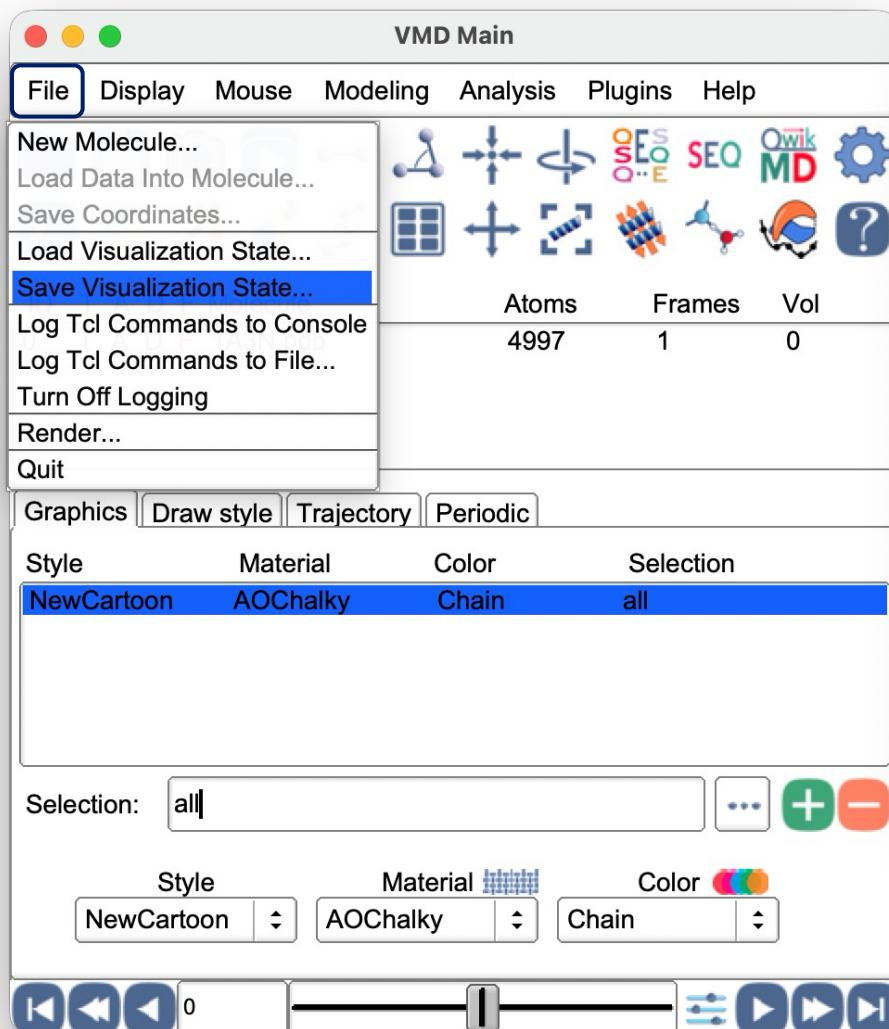


“Fancy” Tachyon



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

Saving current scene



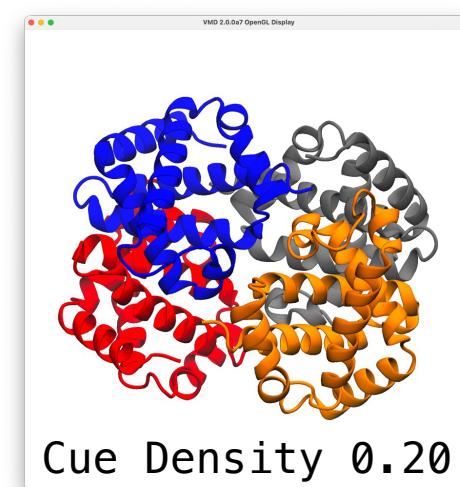
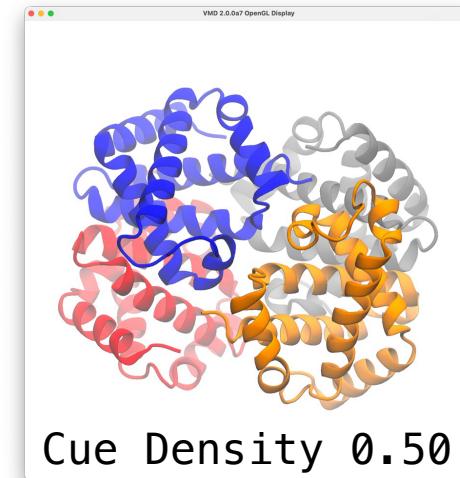
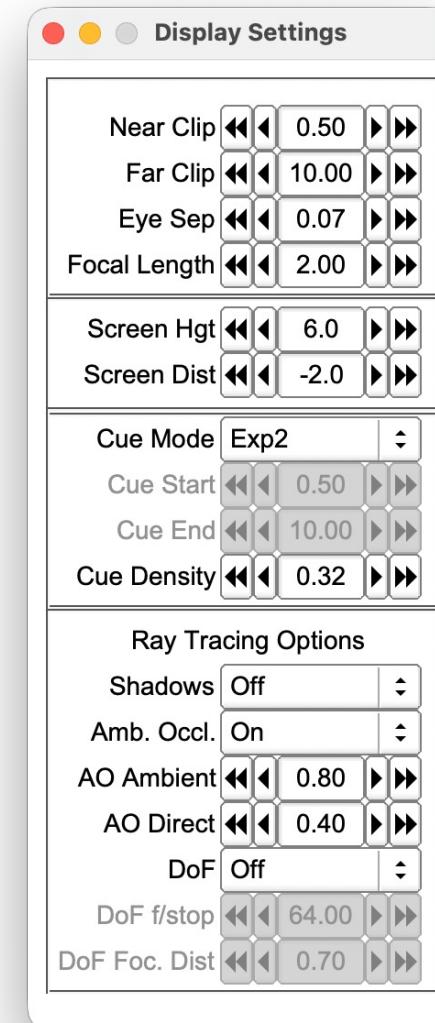
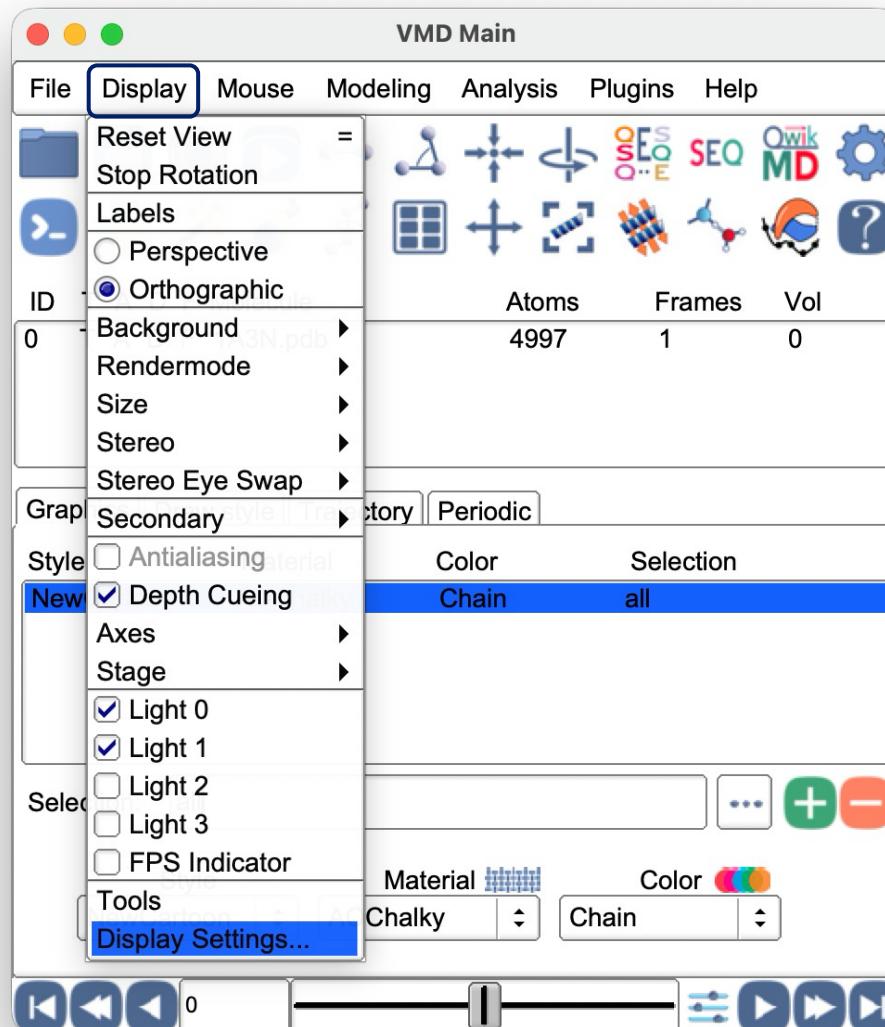
Note that the state file **only references** the topology file. Therefore,

- if the coordinates on the PDB change, the visualization will reflect these changes
- if the path of the PDB changes, the state file will fail to load.



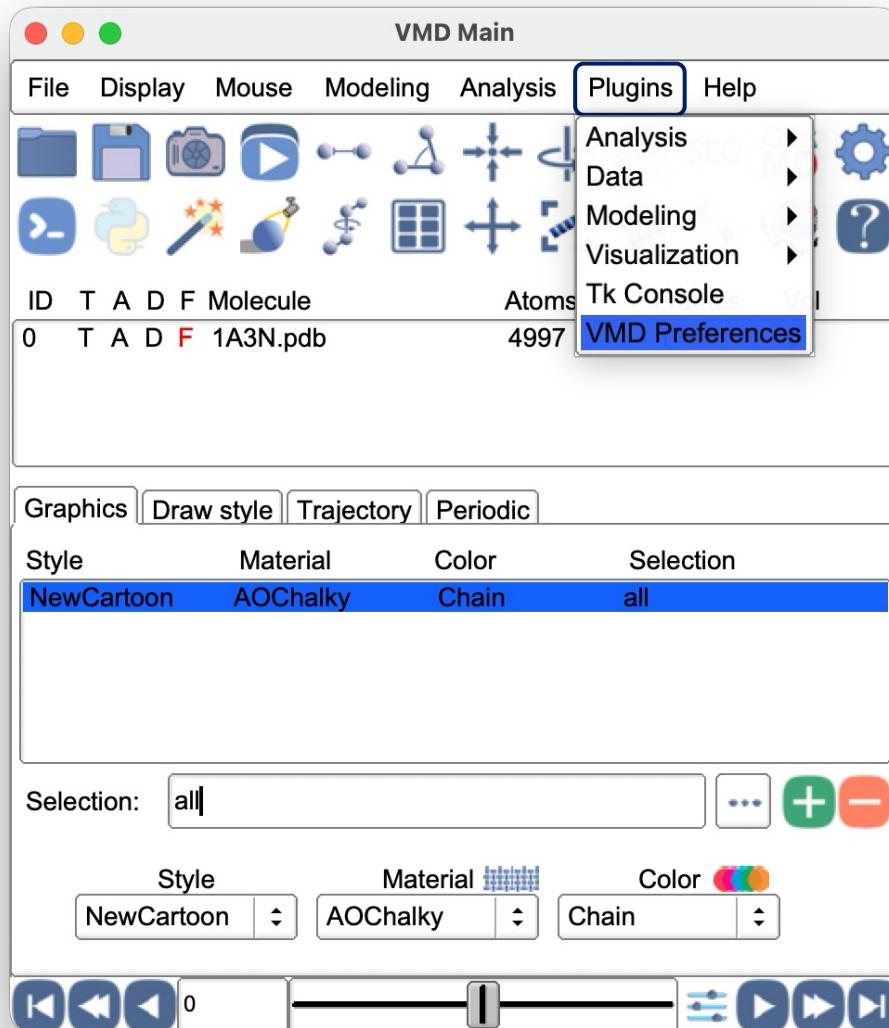
Useful to save the scene of a presentation or publication figure

Advanced options

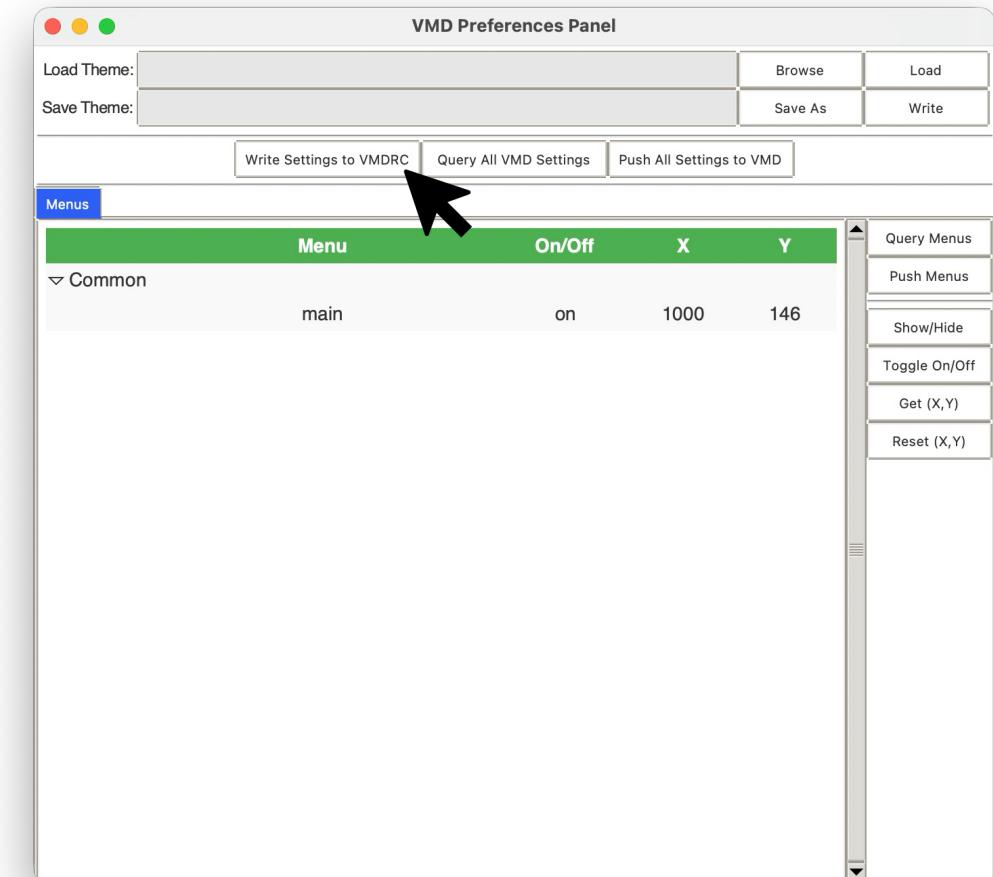


version 2.0.0

Advanced options

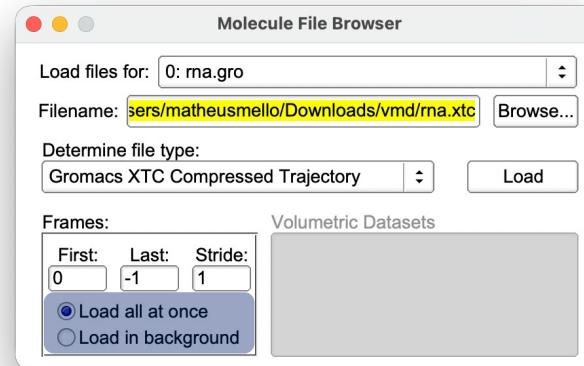
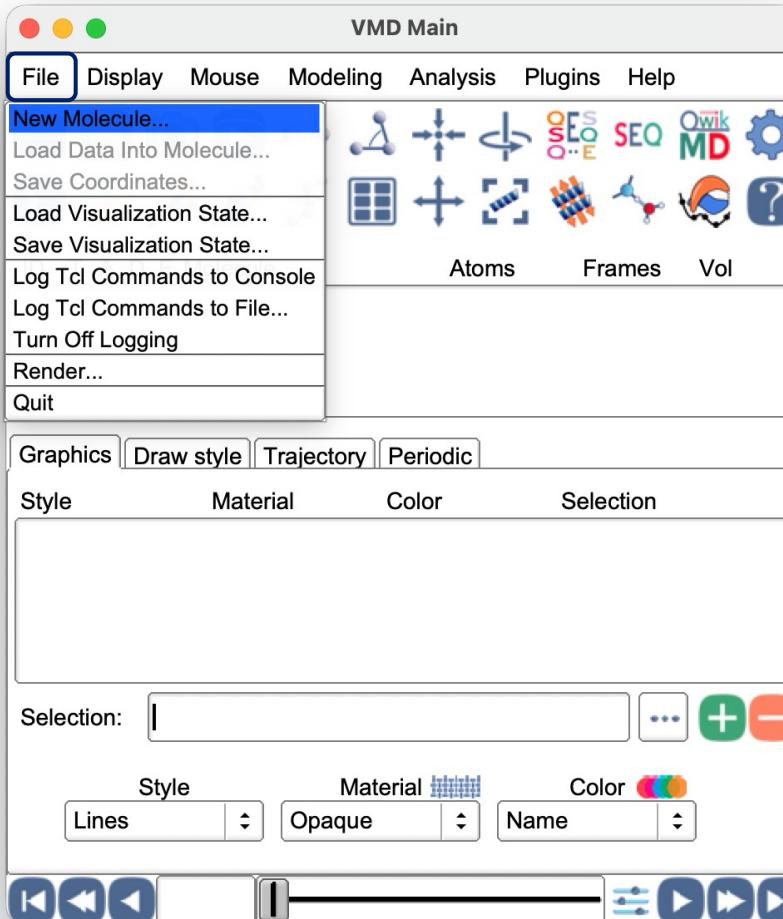


Save current settings, to apply every time VMD opens:



Managing trajectories

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



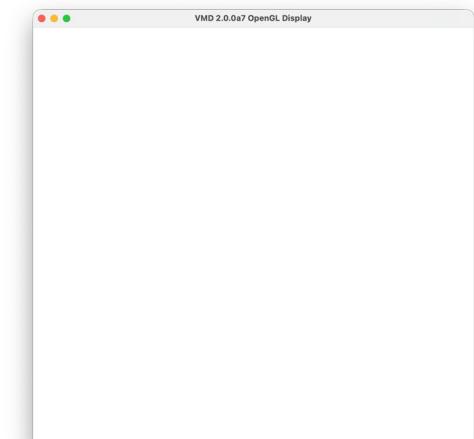
} The trajectory file is loaded on top of the topology file
} Load all at once loads faster, especially for larger systems



Note that the molecule leaves the field of view

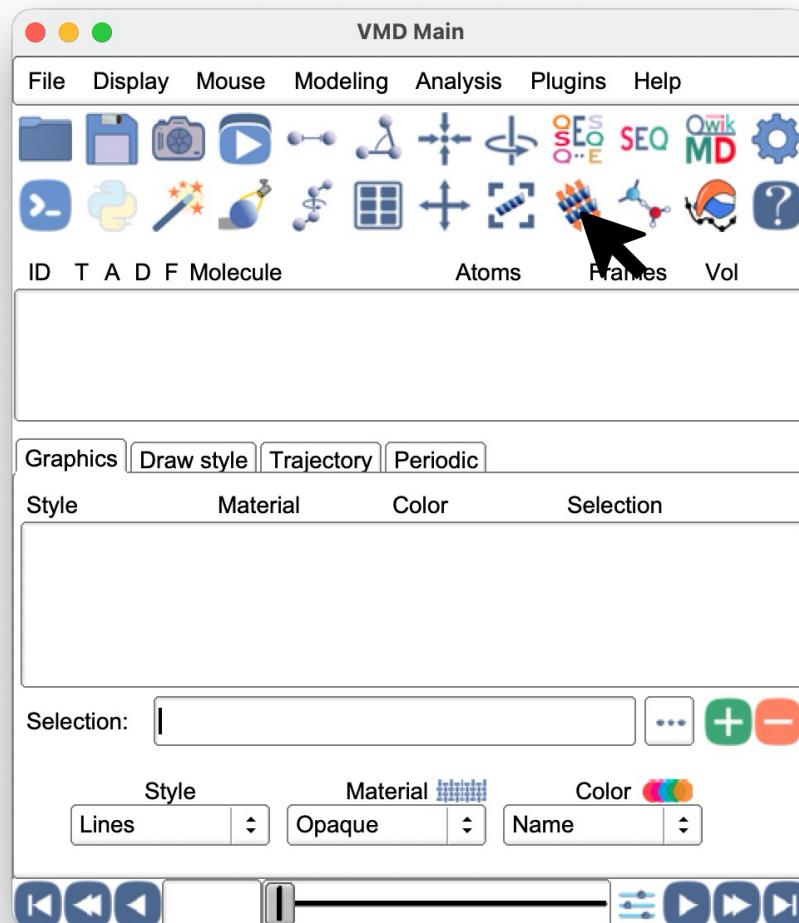
Solutions:

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

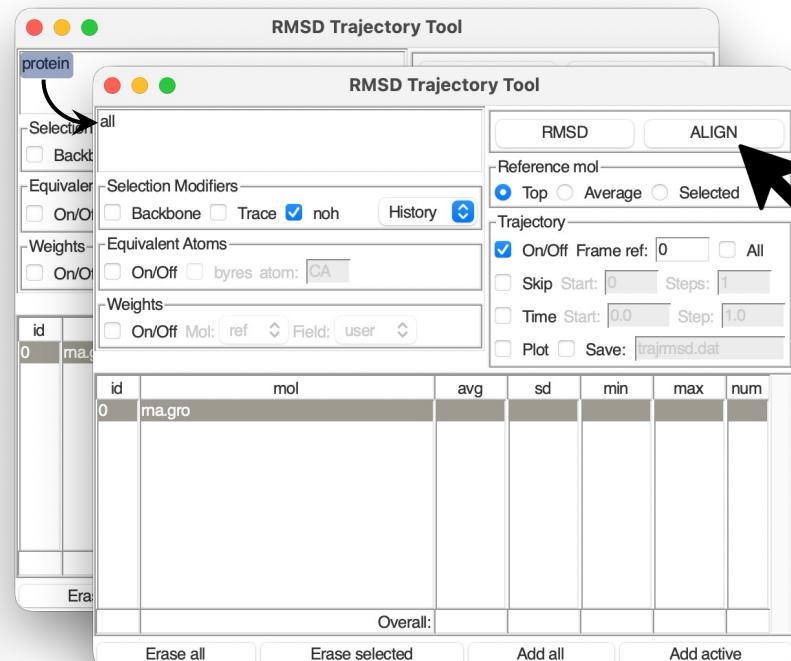


Aligning trajectories

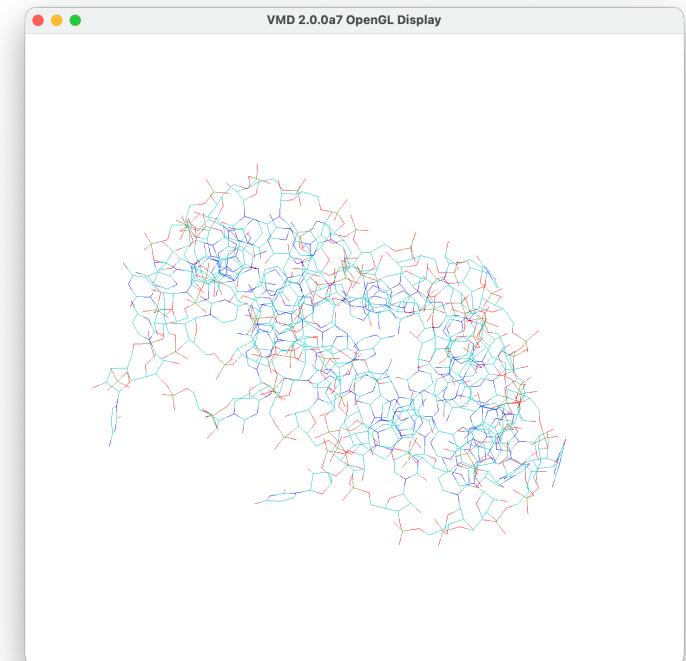
Open RMSD Trajectory tool



Change selection and align



Reset view (=)

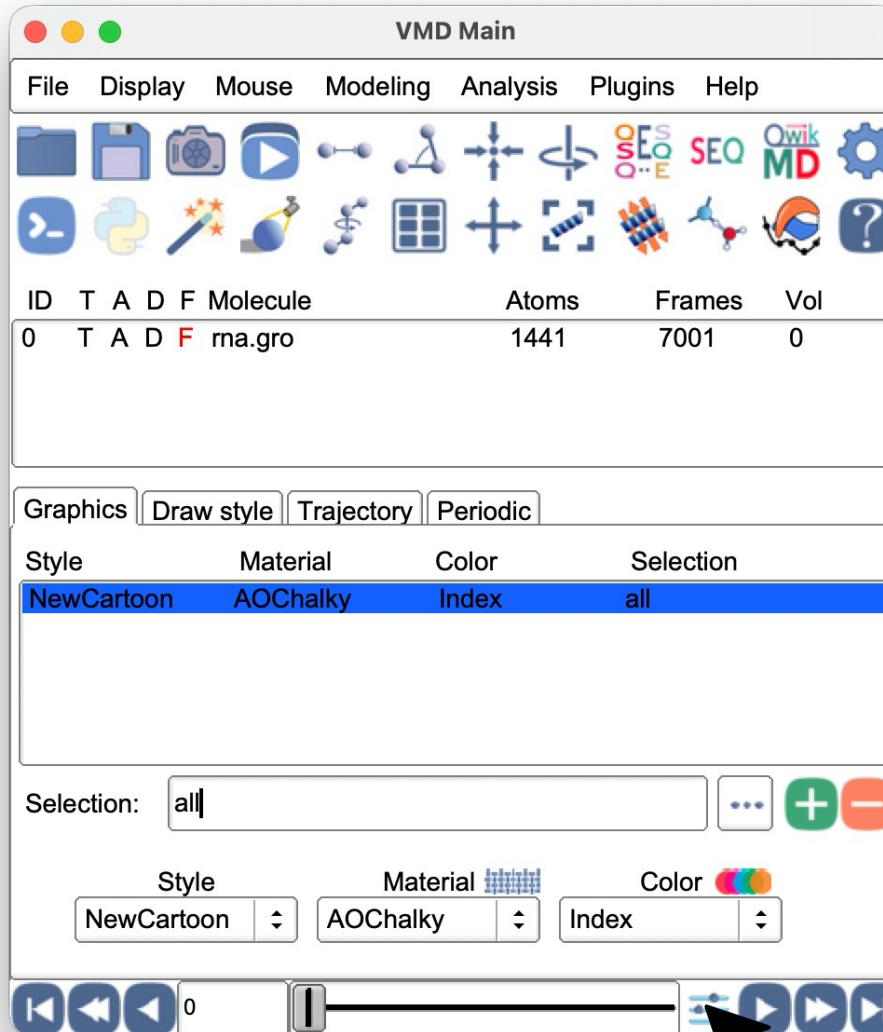


Try a custom selection and explore a representation that you like!

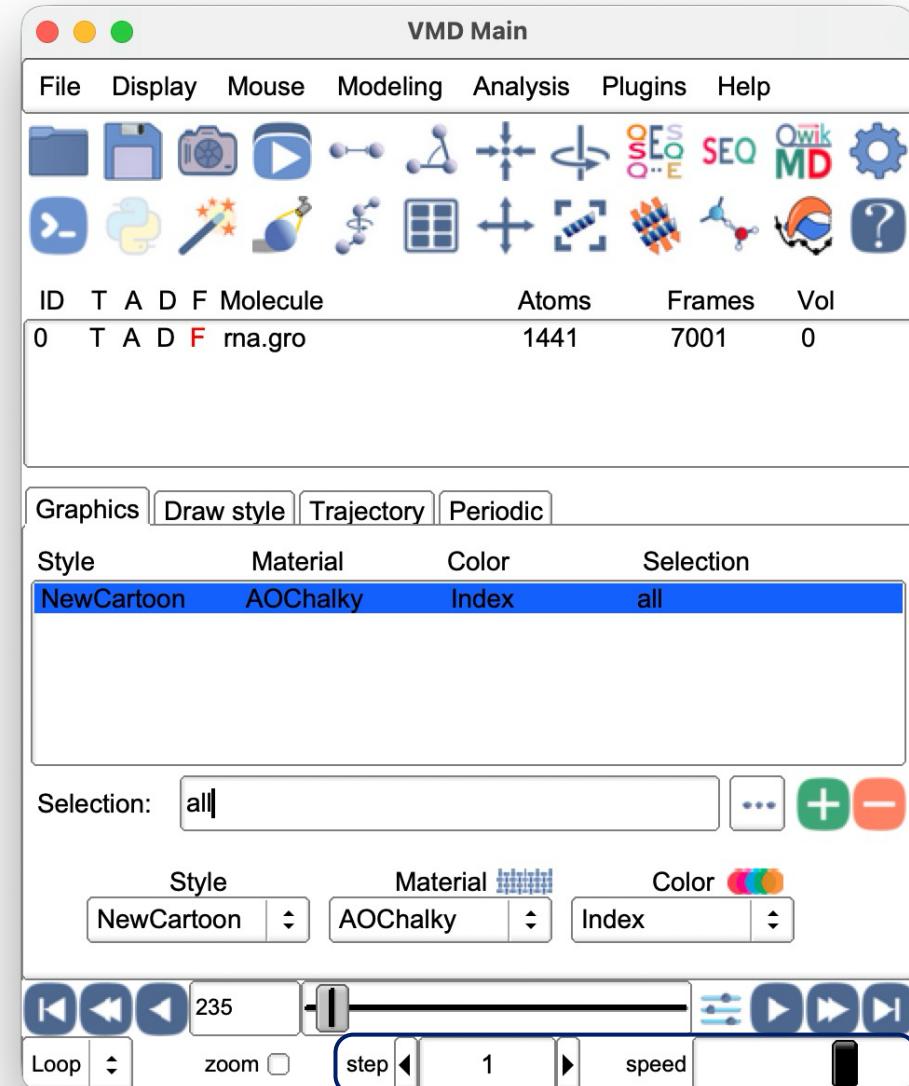
Alternatively : Extensions > Analysis > RMSD Trajectory Tool

version 2.0.0

Managing trajectories

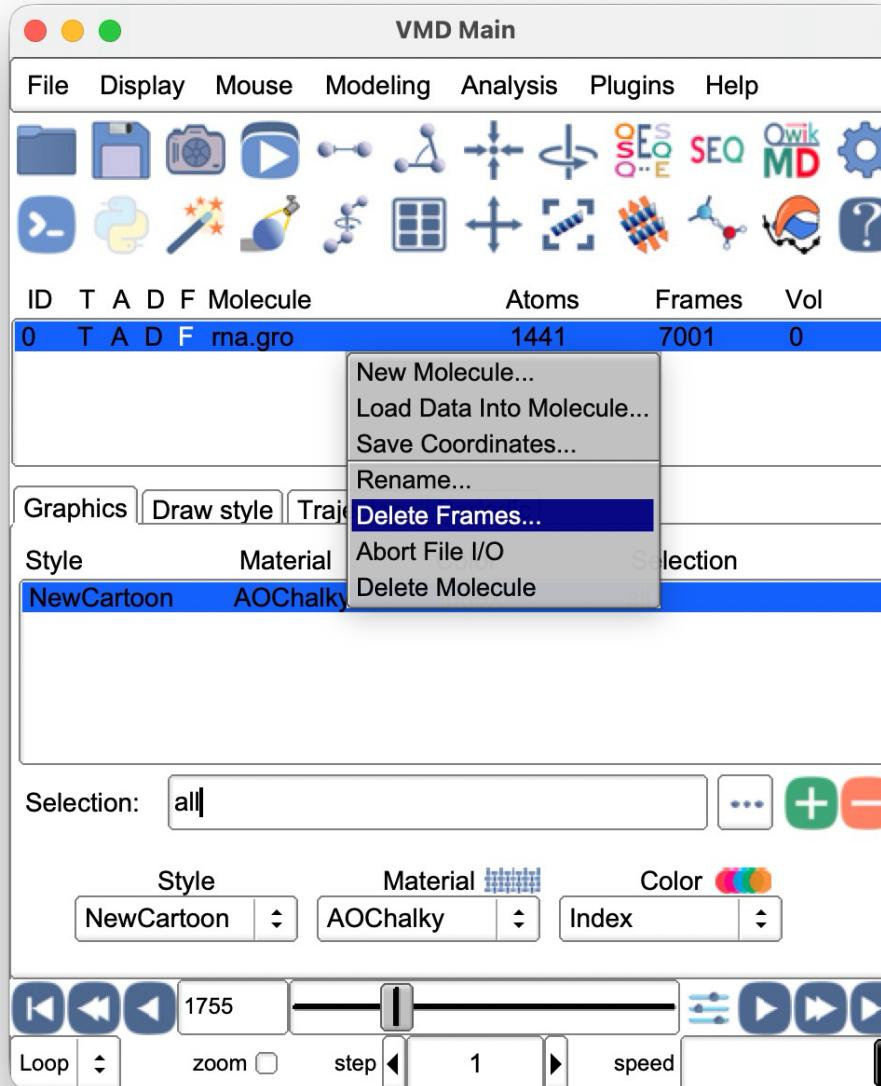


Skip to last frame
Next frame
Play forward

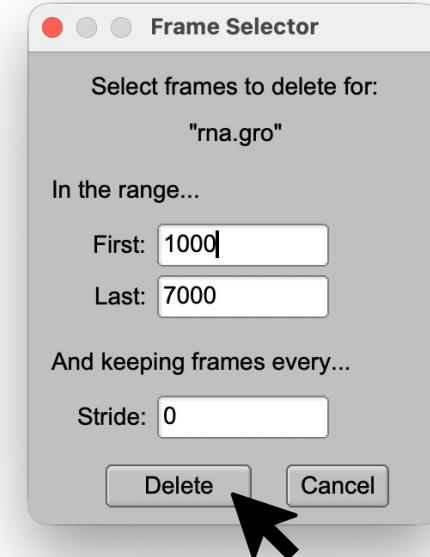


version 2.0.0

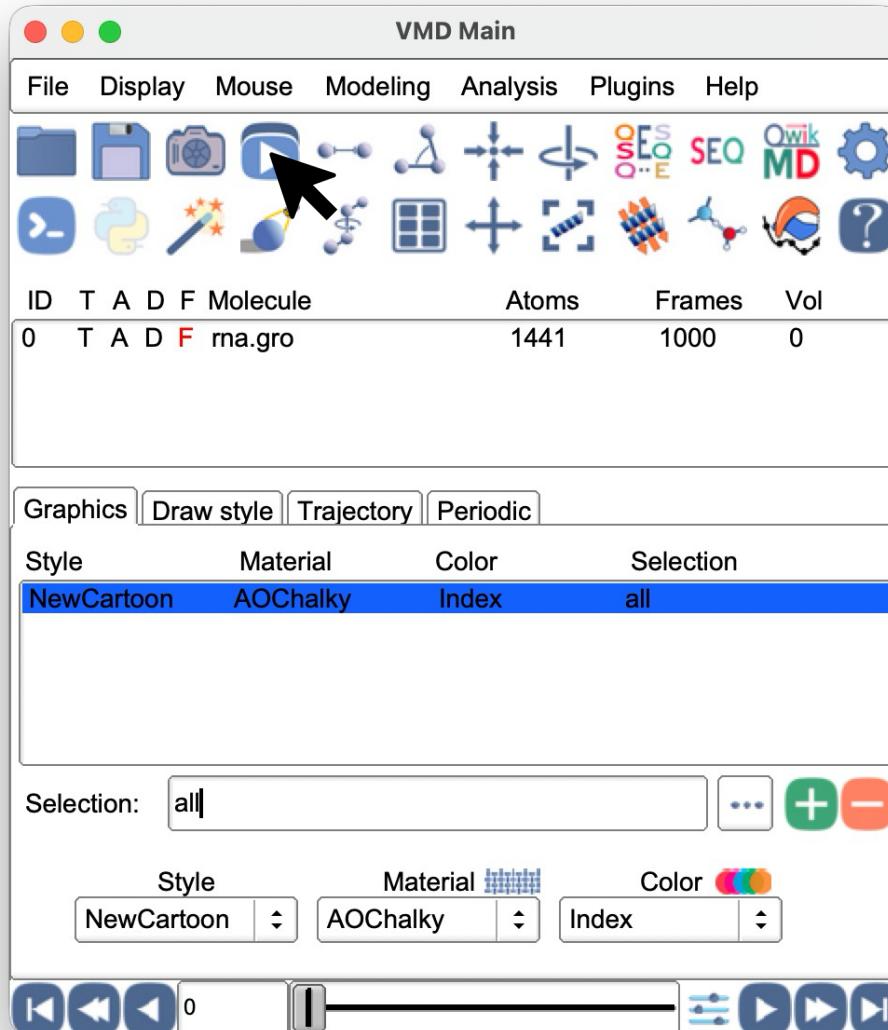
Managing trajectories



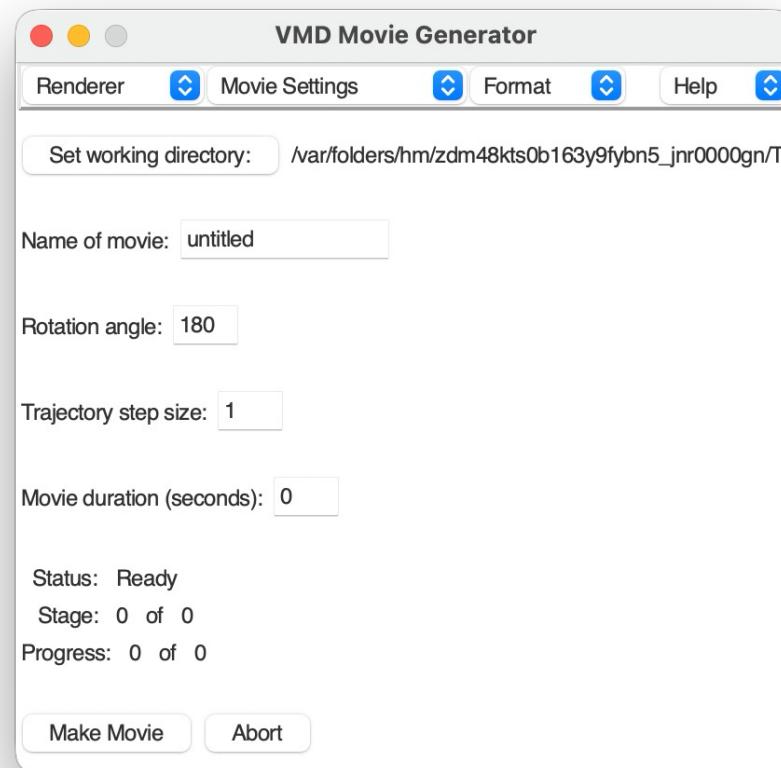
The trajectory is quite long!
Let's keep only the first 1,000 frames.



Rendering videos



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

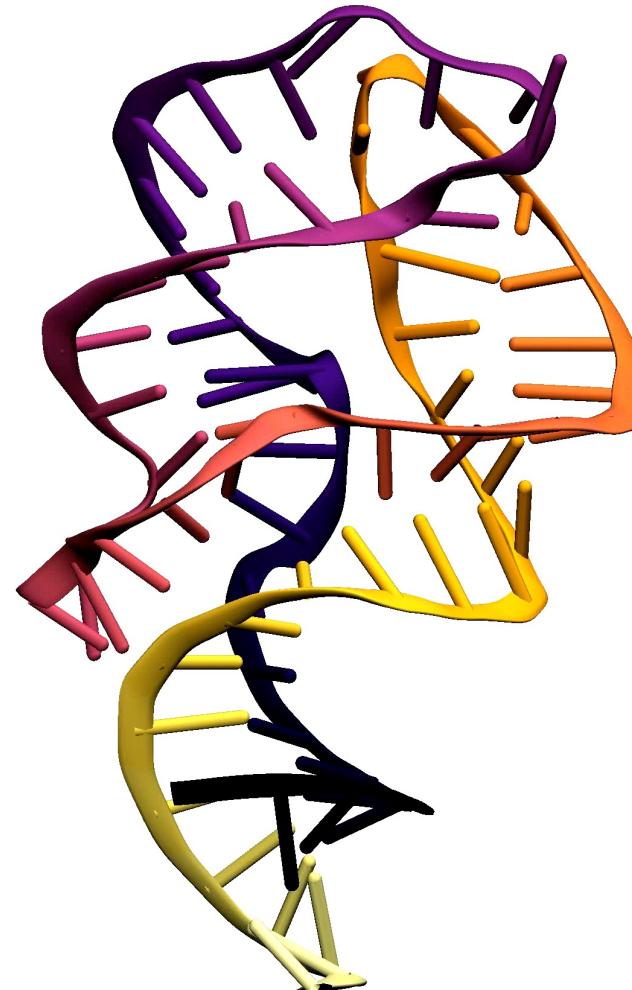


} Set the proper directory
Name your movie

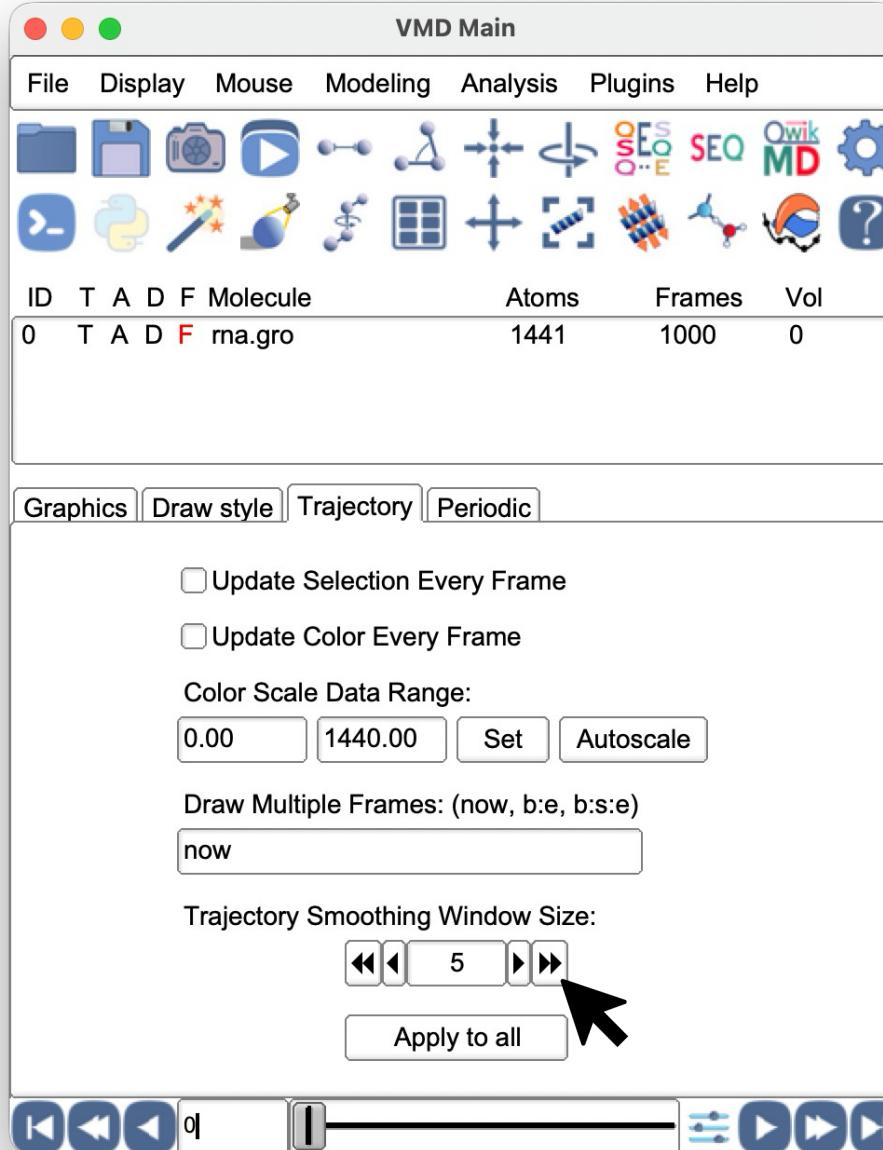
version 2.0.0

Rendering videos

Our results so far...

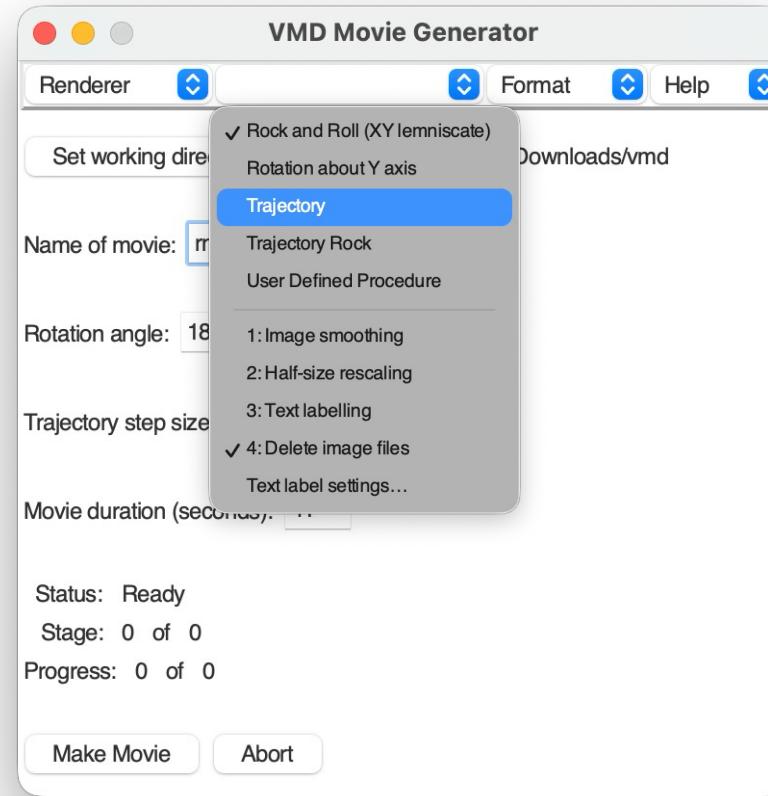


Rendering videos



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?

Additional resources:

- Complete list of selection keywords: <https://www.ks.uiuc.edu/Research/vmd/vmd-1.7.1/ug/node79.html>
- VMD mailing list: https://www.ks.uiuc.edu/Research/vmd/mailing_list/
- VMD manual and tutorials: <https://www.ks.uiuc.edu/Research/vmd/current/docs.html>
- Tutorial on Ambient Occlusion and Transparency with Tachyon:
https://mini.ourphysics.org/wiki/index.php/How_to_make_images_for_publication_using_VMD.html

