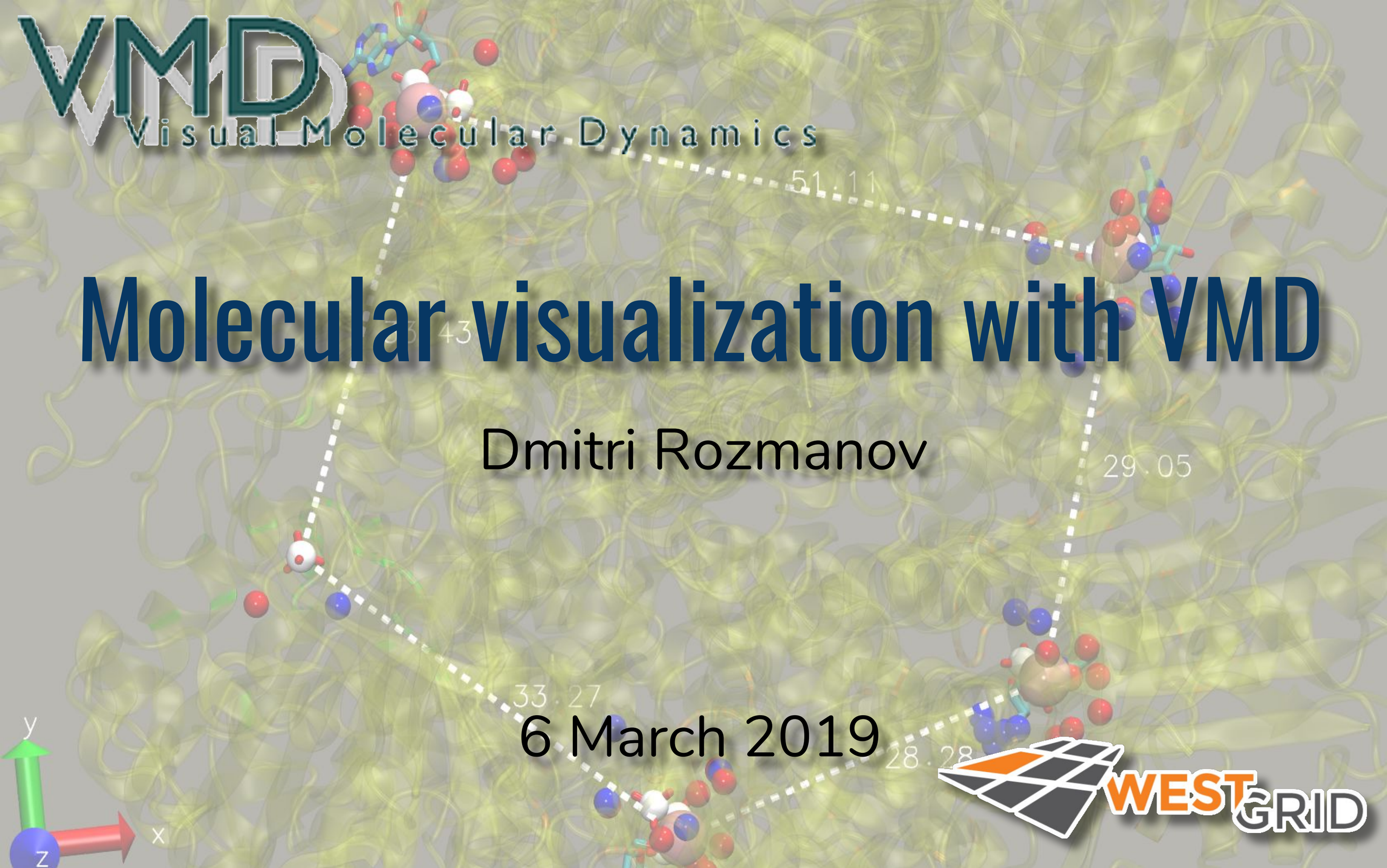


Molecular visualization with VMD

Dmitri Rozmanov

6 March 2019

WESTGRID

What is VMD ?

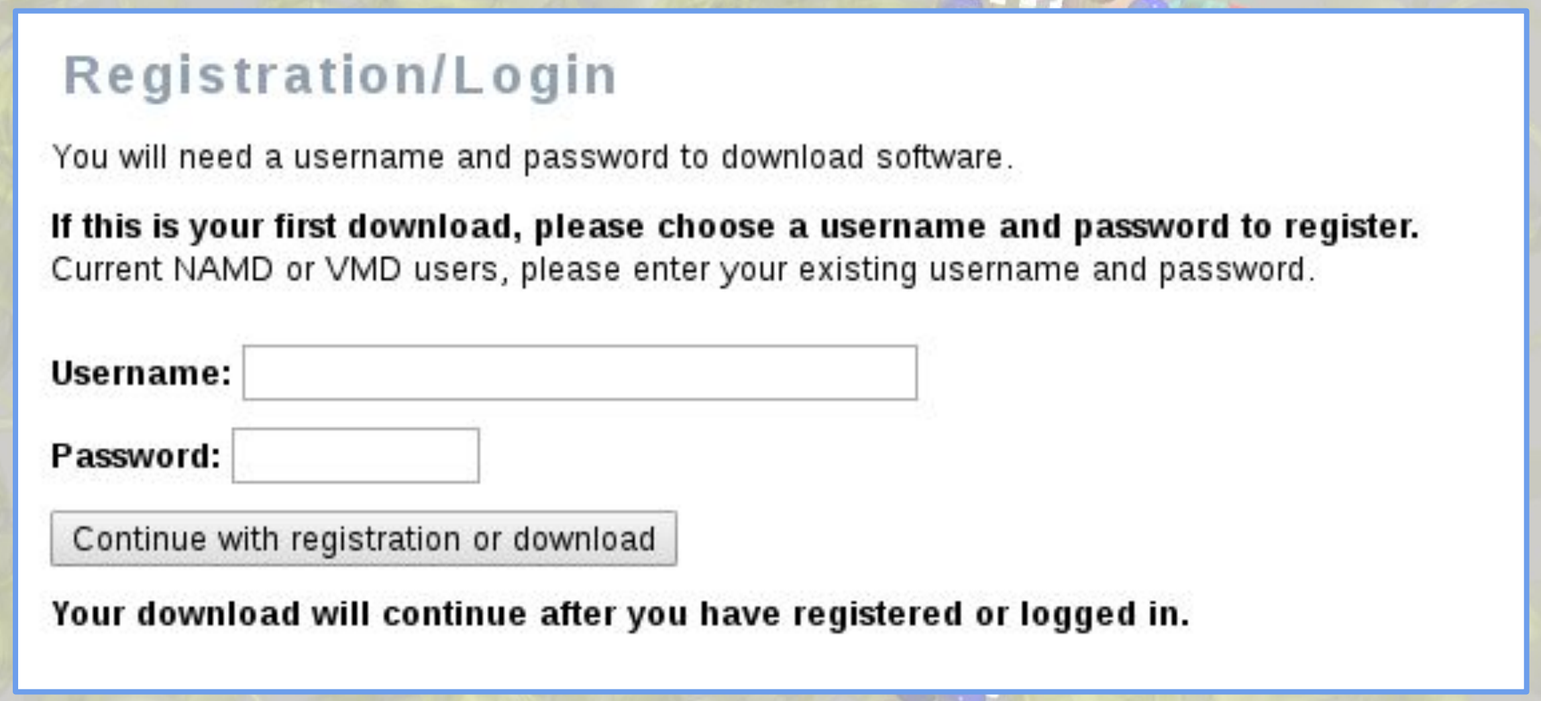
Visual Molecular Dynamics (VMD) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

Features:

- Distributed **free** of charge, and includes source code.
- Available for MacOS, Unix, or Windows.
- **Very fast**, written in C++.
  Supports Multi-core CPUs, GPUs, and CUDA.
- Tcl/Tk and Python **scripting**.
- Supports over 60 molecular **file formats** and data types.
- Publication **quality** image rendering.

Getting VMD

Download:
https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD



Citing VMD

Humphrey, W., Dalke, A. and Schulten, K., ”VMD - Visual Molecular Dynamics”, J. Molec. Graphics, 1996, vol. 14, pp. 33-38.

Also see: http://www.ks.uiuc.edu/Research/vmd/allversions/cite.html

Overview of VMD related topics

- **Basic techniques**
  - **Molecules and representations.**
  - **3D navigation.**
  - **Drawing methods.**
  - **Materials and coloring.**
  - **Atom selection techniques.**
- Working with trajectories.
- Creating animations and movies.
- Scripting and automation.
- **Rendering high quality images.**
- Data analysis.
- Visualization of volumetric data.
- Running VMD in HPC environment.

Starting VMD

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID T A D F Molecule Atoms Frames Vol

zoom Loop step 1 speed

Main control window

VMD 1.9.3 OpenGL Display

VMD

Theoretical and Computational Biophysics Group
NIH Resource for Macromolecular Modeling and Bioinformatics
University of Illinois at Urbana-Champaign
R. Brunner, E. Caddigan, J. Cohen, A. Dalke, P. Grayson,
J. Gullingsrud, D. Hardy, W. Humphrey, B. Isralewitz, S. Izrailev,
A. Kohlmeyer, D. Norris, J. Saam, J. Stone, J. Ulrich, K. Vandivort

y x z

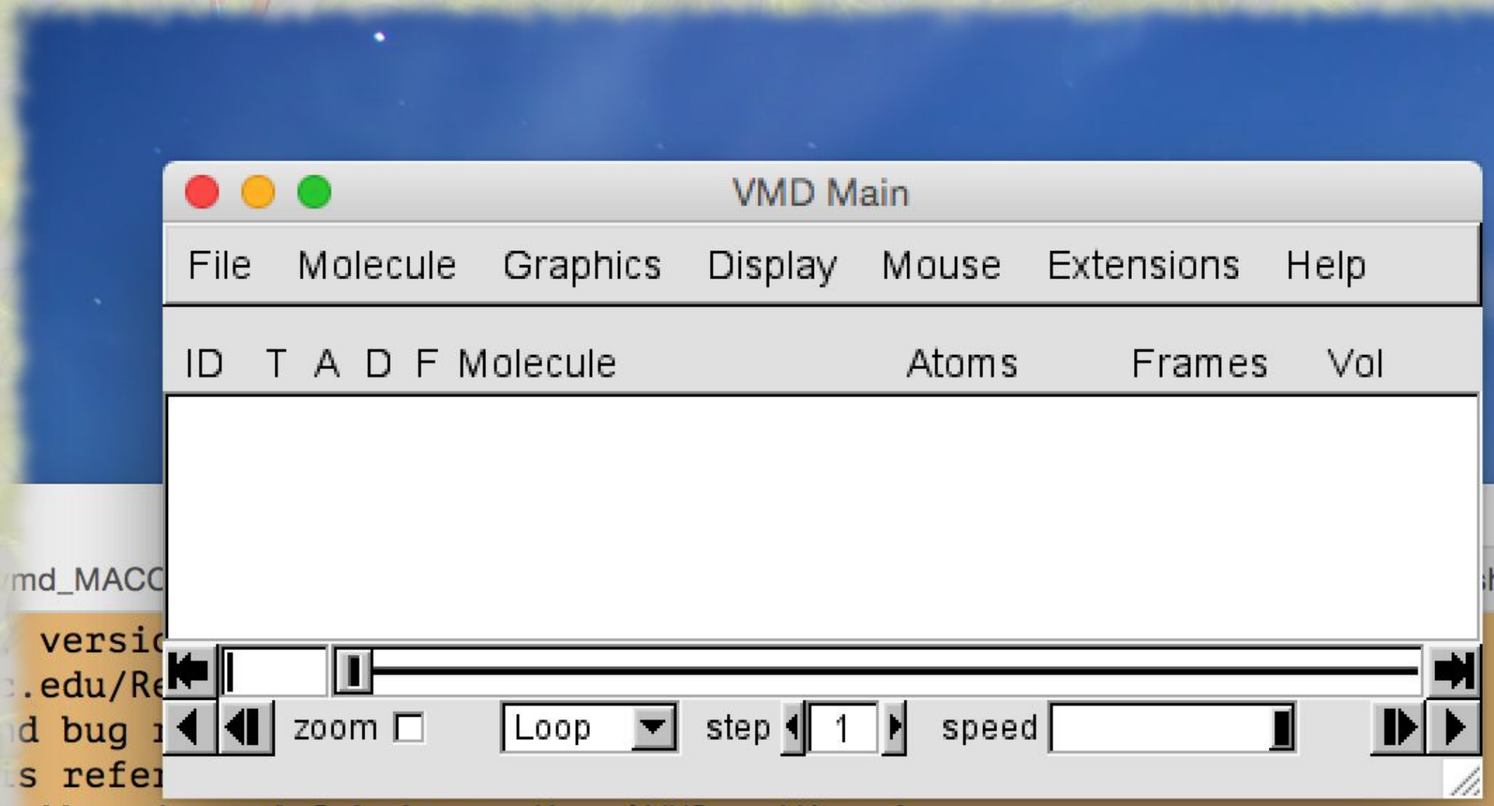
OpenGL graphics window

```
Dalke, A. and Schulten, K., `VMD - Visual
mics', J. Molec. Graphics 1996, 14.1, 33-38.
----------------------------------------
ailable, 8 CPUs detected.
NVIDIA GeForce GT 750M OpenGL Engine
IL MDE CVA MTX NPOT PP PS GLSL(OVF)
ring mode is available.
16384x16384), 3-D (2048x2048x2048), Multitexture (8)
d 2 plugins in directory:
 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile

, version 1.9.3 (November 30, 2016)
Info) Exiting normally.
Dmitris-MacBook-Pro:~ rozmanov$ vmd
Info) VMD for MACOSXX86, version 1.9.3 (November 30, 2016)
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, 8 CPUs detected.
Info) OpenGL renderer: NVIDIA GeForce GT 750M OpenGL Engine
Info)   Features: STENCIL MDE CVA MTX NPOT PP PS GLSL(OVF)
Info)   Full GLSL rendering mode is available.
Info)   Textures: 2-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
Info) Dynamically loaded 2 plugins in directory:
Info) /Applications/VMD 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile
vmd >
```

Terminal window

Main control



Display

- Reset View =
- Stop Rotation
- (•) Perspective
- ( ) Orthographic
- [ ] Antialiasing
- [x] Depth Cueing
- [ ] Culling
- [ ] FPS Indicator
- [x] Light 0
- [x] Light 1
- [ ] Light 2
- [ ] Light 3
- Axes ▸
- Background ▸
- Stage ▸
- Stereo ▸
- Stereo Eye Swap ▸
- Cachemode ▸
- Rendermode ▸
- Display Settings...

File

- 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

Molecule

- Make Top
- Toggle Active
- Toggle Displayed
- Toggle Fixed
- Rename...
- Delete Frames...
- Abort File I/O
- Delete Molecule

Graphics

- Representations...
- Colors...
- Materials...
- Labels...
- Tools...

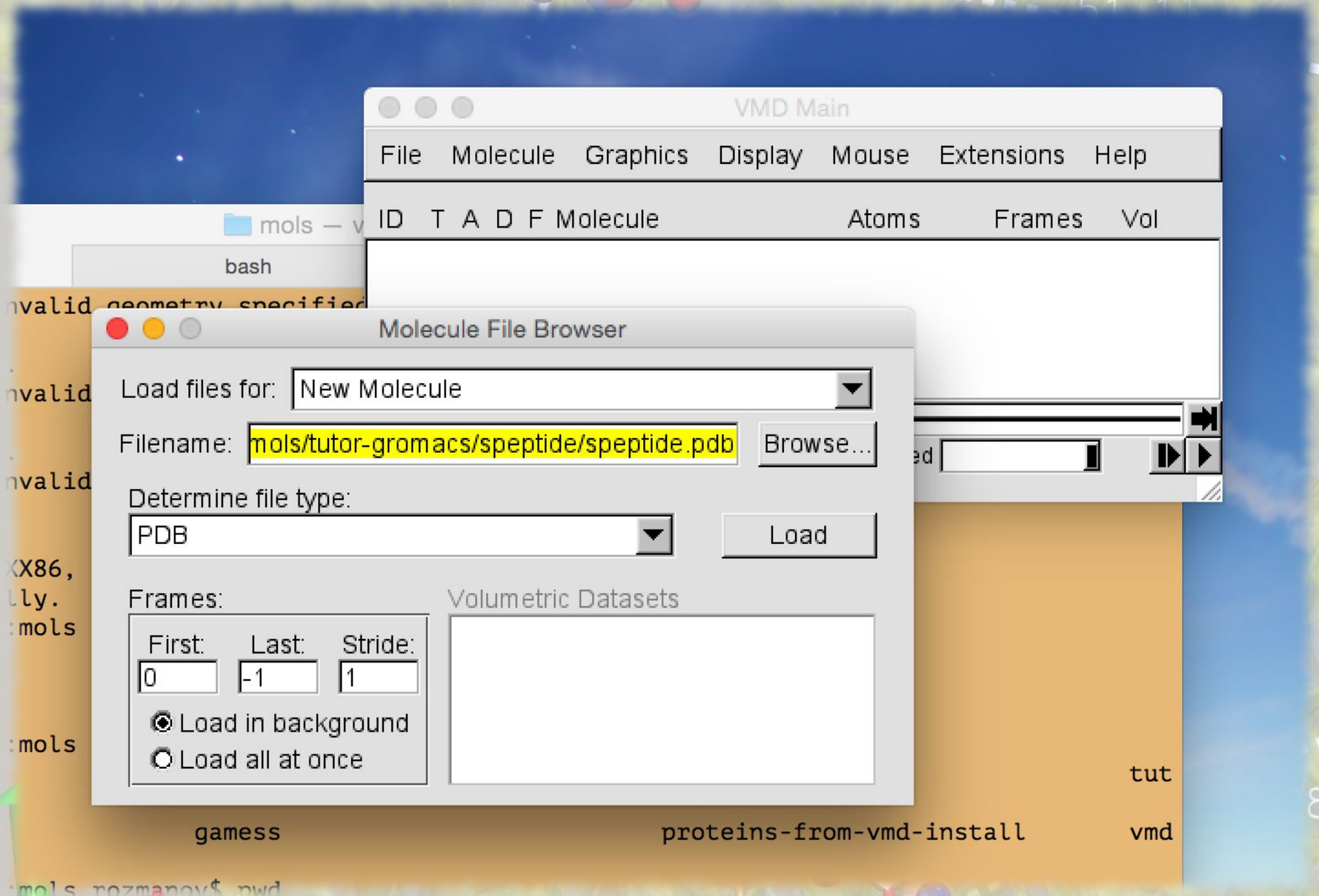
Mouse

- (•) Rotate Mode R
- ( ) Translate Mode T
- ( ) Scale Mode S
- ( ) Center C
- ( ) Query 0
- [ ] Label ▸
- [ ] Move ▸
- [ ] Force ▸
- [ ] Move Light ▸
- ( ) Add/Remove Bonds
- ( ) Pick P

Extensions

- Analysis ▸
- Data ▸
- Modeling ▸
- Simulation ▸
- Visualization ▸
- Tk Console
- VMD Preferences

Loading a new molecule



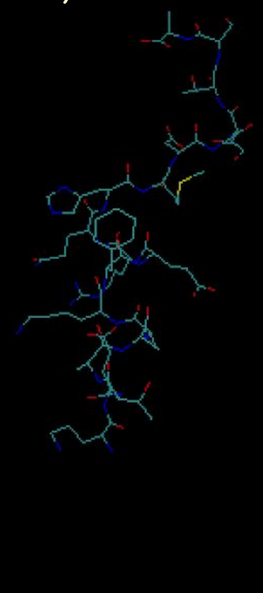
1. Load for a **New Molecule**.
2. Determine type **Automatically**.
3. Select file **speptide.pdb**
4. Click **Load**.
5. Close the **dialog**.

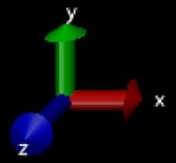
Loading a molecule

VMD 1.9.3 OpenGL Display

Short Peptide:

- 146 atoms;
- 18 residues;





Loaded molecule

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

zoom Loop step 1 speed

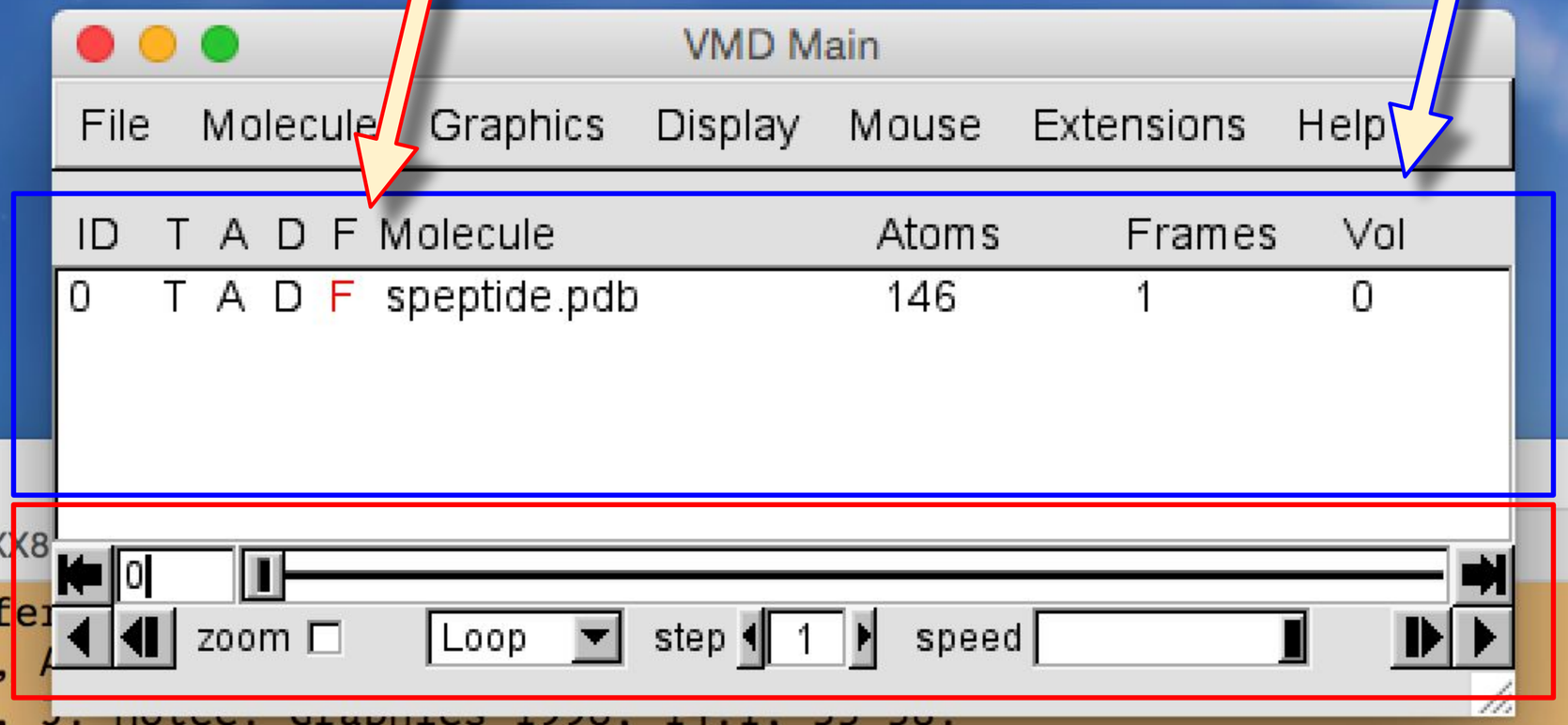
Loaded molecule

```
vmd_MACOSXX8
e this refe
W., Dalke, A
Dynamics', J. Molec. Graphics 1996, 14.1, 33-38.
------------------------------------------------
g available, 8 CPUs detected.
er: NVIDIA GeForce GT 750M OpenGL Engine
TENCIL MDE CVA MTX NPOT PP PS GLSL(OVF)
endering mode is available.
-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
oaded 2 plugins in directory:
/VMD 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile
lugin pdb for structure file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tut
/speptide.pdb
Info) Using plugin pdb for coordinates from file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tu
tor-gromacs/speptide/speptide.pdb
Info) Determining bond structure from distance search ...
Info) Analyzing structure ...
Info)    Atoms: 146
Info)    Bonds: 147
Info)    Angles: 0  Dihedrals: 0  Impropers: 0  Cross-terms: 0
Info)    Bondtypes: 0  Angletypes: 0  Dihedraltypes: 0  Impropertypes: 0
Info)    Residues: 19
Info)    Waters: 0
Info)    Segments: 1
Info)    Fragments: 1   Protein: 1   Nucleic: 0
Info) Finished with coordinate file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tutor-gromacs/s
peptide/speptide.pdb.
```

Main control window

List of molecules

"Red" means **inactive**



Trajectory animation controls

ID - molecule number.

T - "Top" stat.

A - Active.

D - Drawn.

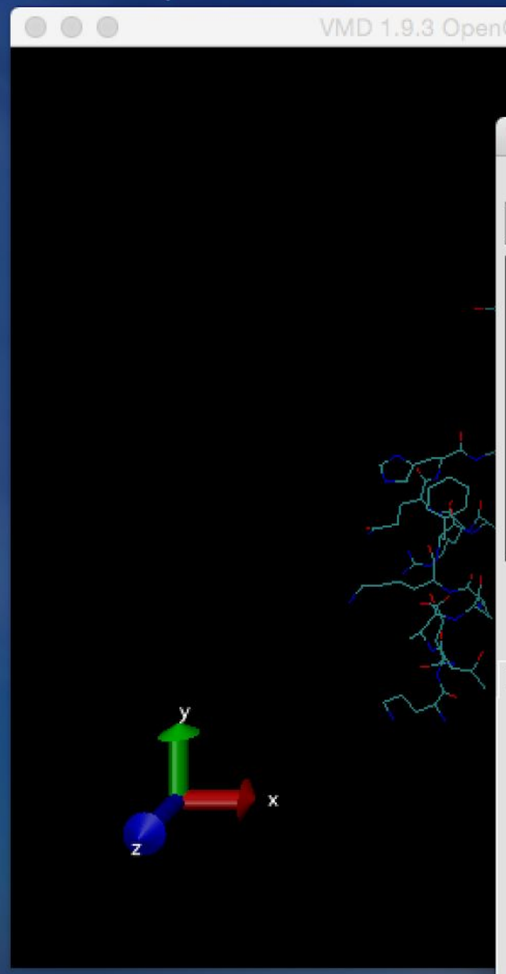
F - Fixed.

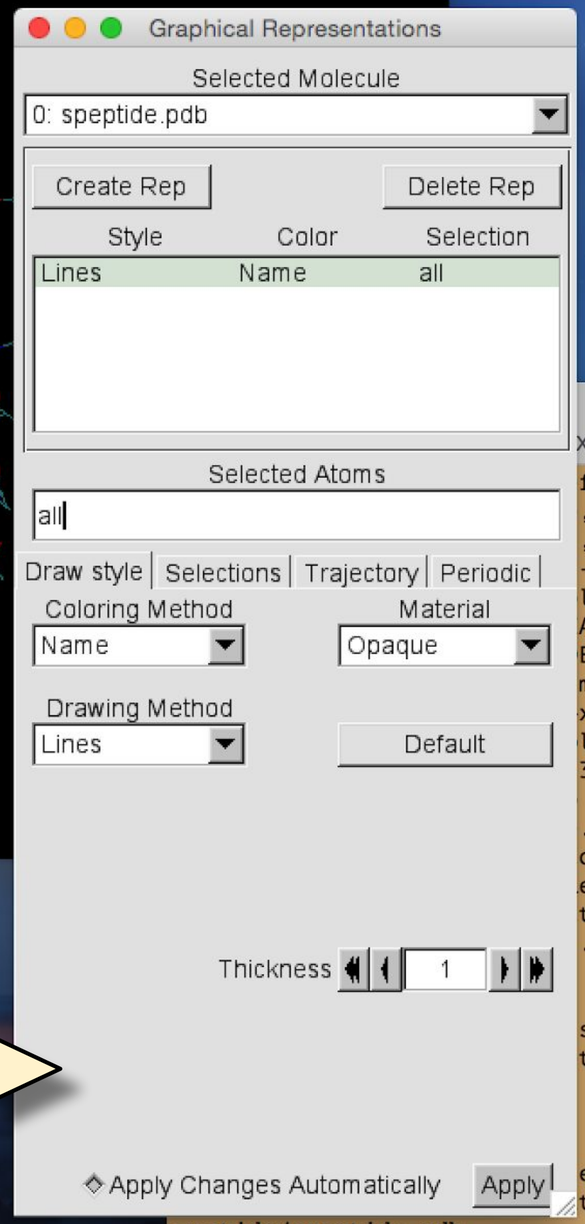
of **Atoms**.

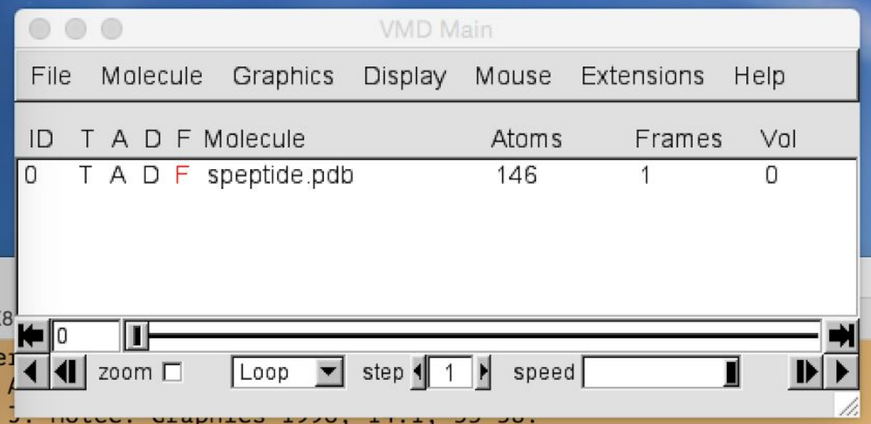
of **Frames**.

Volumetric data.

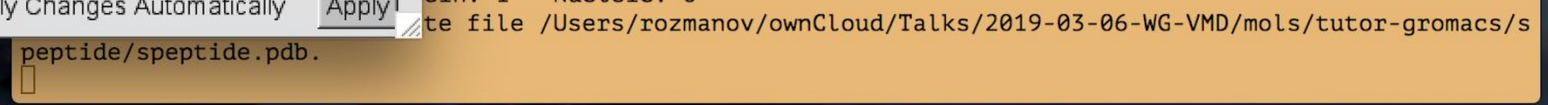
Working with a single molecule







Graphical Representations window



Representations

- Atom selection
- Drawing method
- Coloring method
- Material

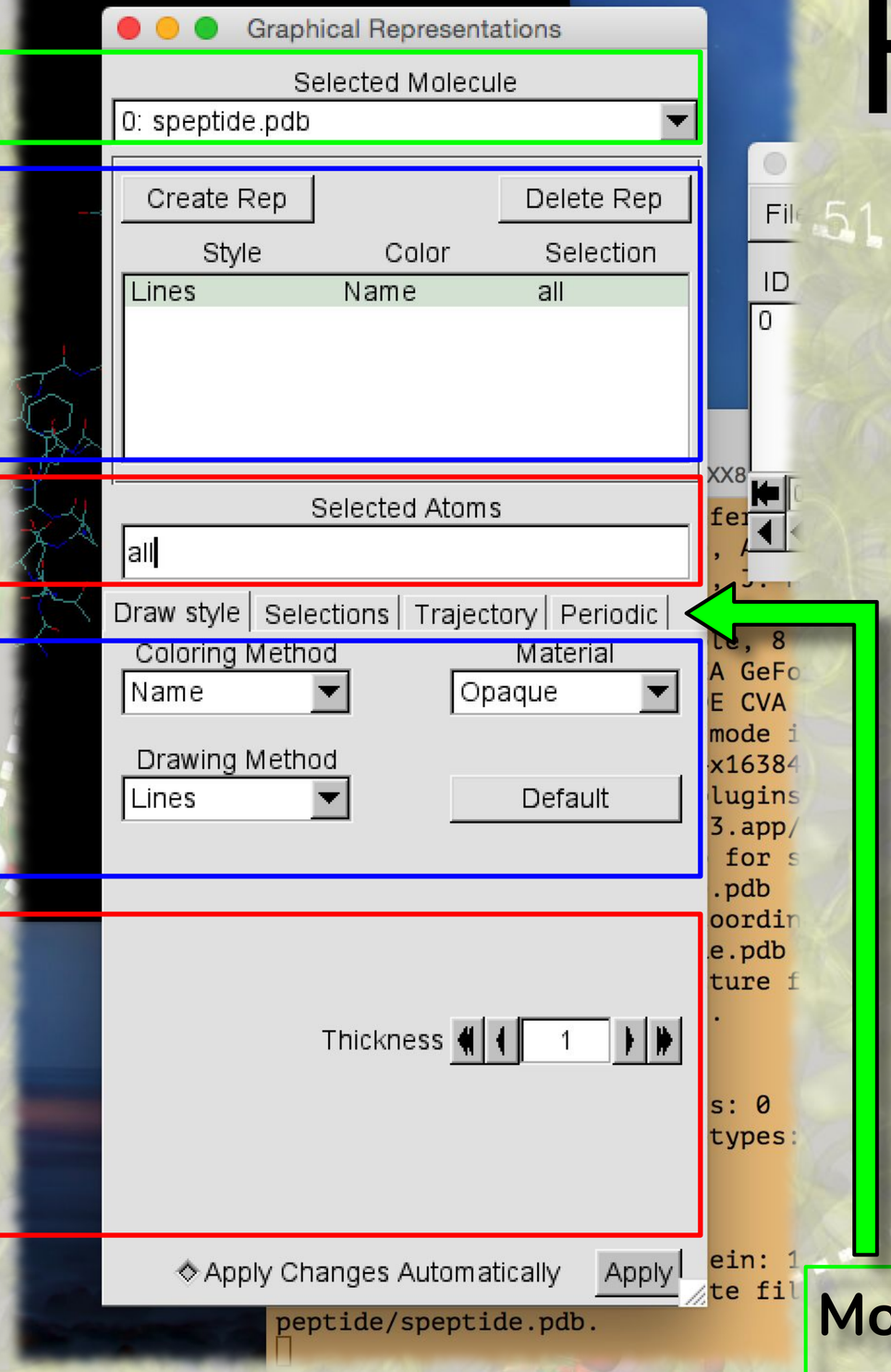
Molecule selector.

List of Representations.

Atom selection.

Drawing method, Coloring scheme, Material controls.

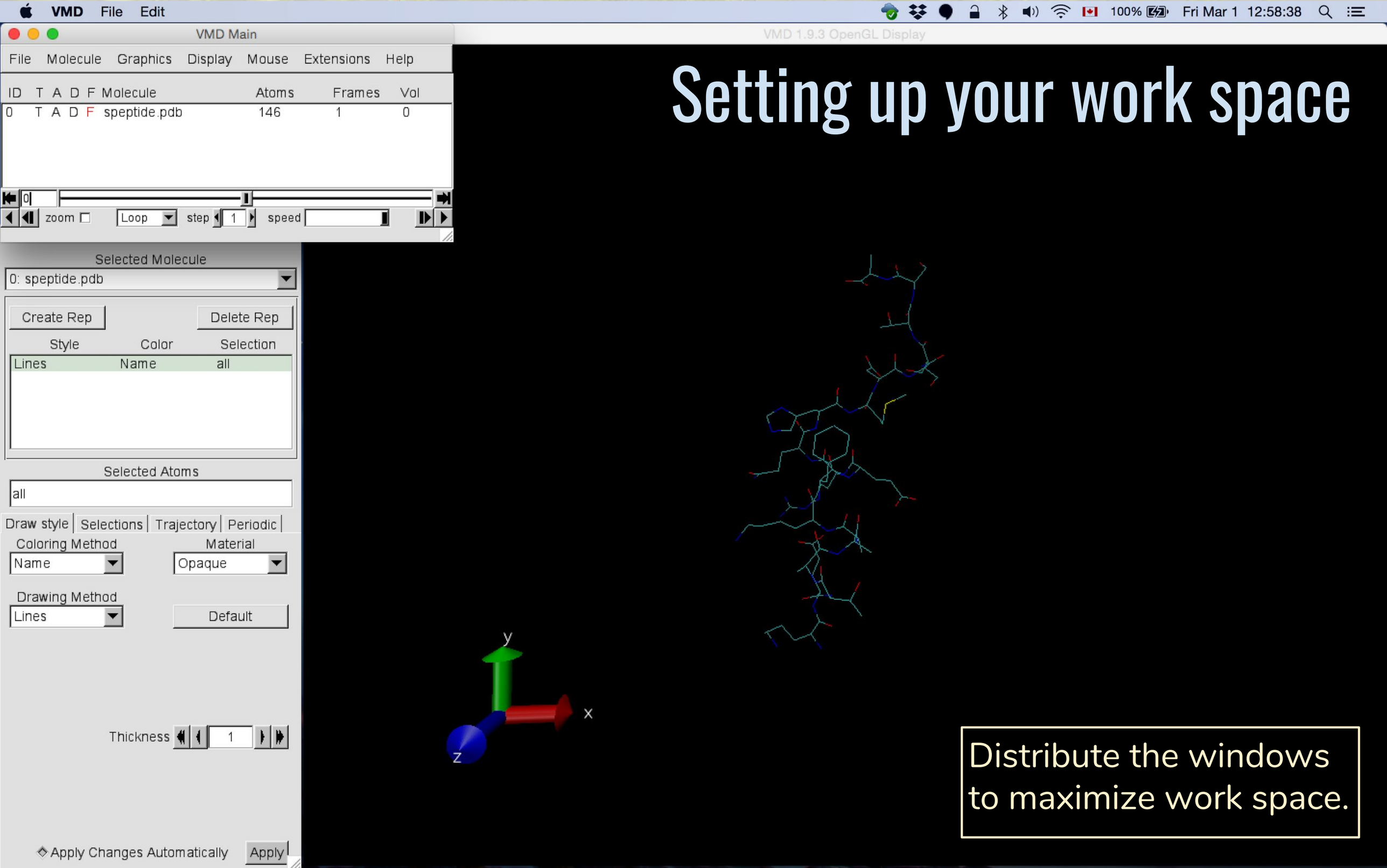
Drawing method parameters.



A molecule can have multiple representations.

More options

Setting up your work space



Distribute the windows to maximize work space.

Setting up work space

VMD File Edit — 100% Fri Mar 1 13:01:53

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

0 zoom Loop step 1 speed

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style Color Selection

Lines Name all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name — Material: Opaque

Drawing Method: Lines — Default

Thickness 1

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

Color Controls

Assign colors to categories:

Categories	Names	Colors
Display	Background	0 blue
Axes	BackgroundTop	1 red
Name	BackgroundBot	2 gray
Type	Foreground	3 orange
Element	FPS	4 yellow
Resname		5 tan

Color Definitions | Color Scale

0 blue
1 red
2 gray
3 orange
4 yellow
5 tan

0.35
0.35
0.35

Grayscale Default

y x z

Colours control window

Colour control

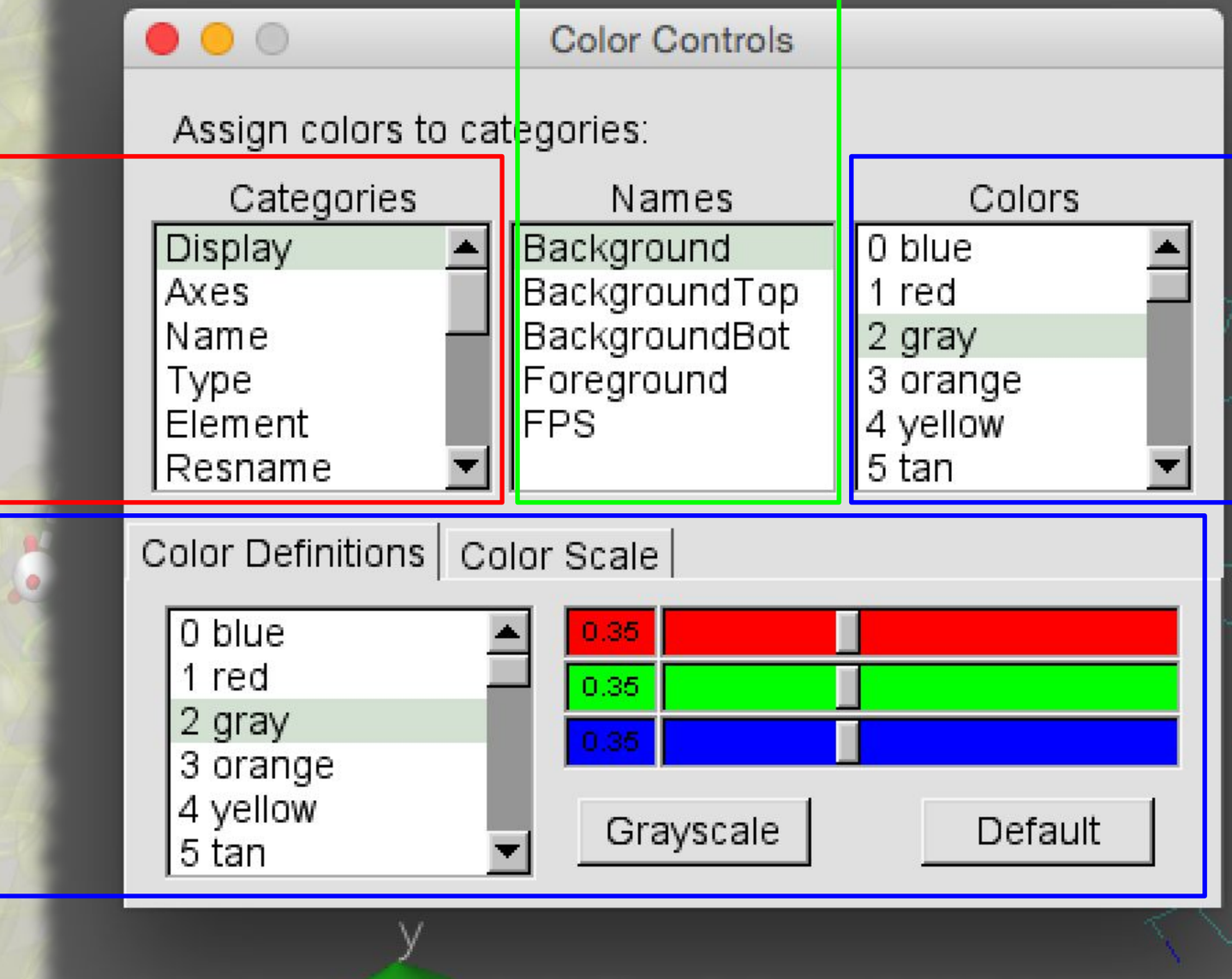
Floating dialog.
Stays until closed.

Items and Objects

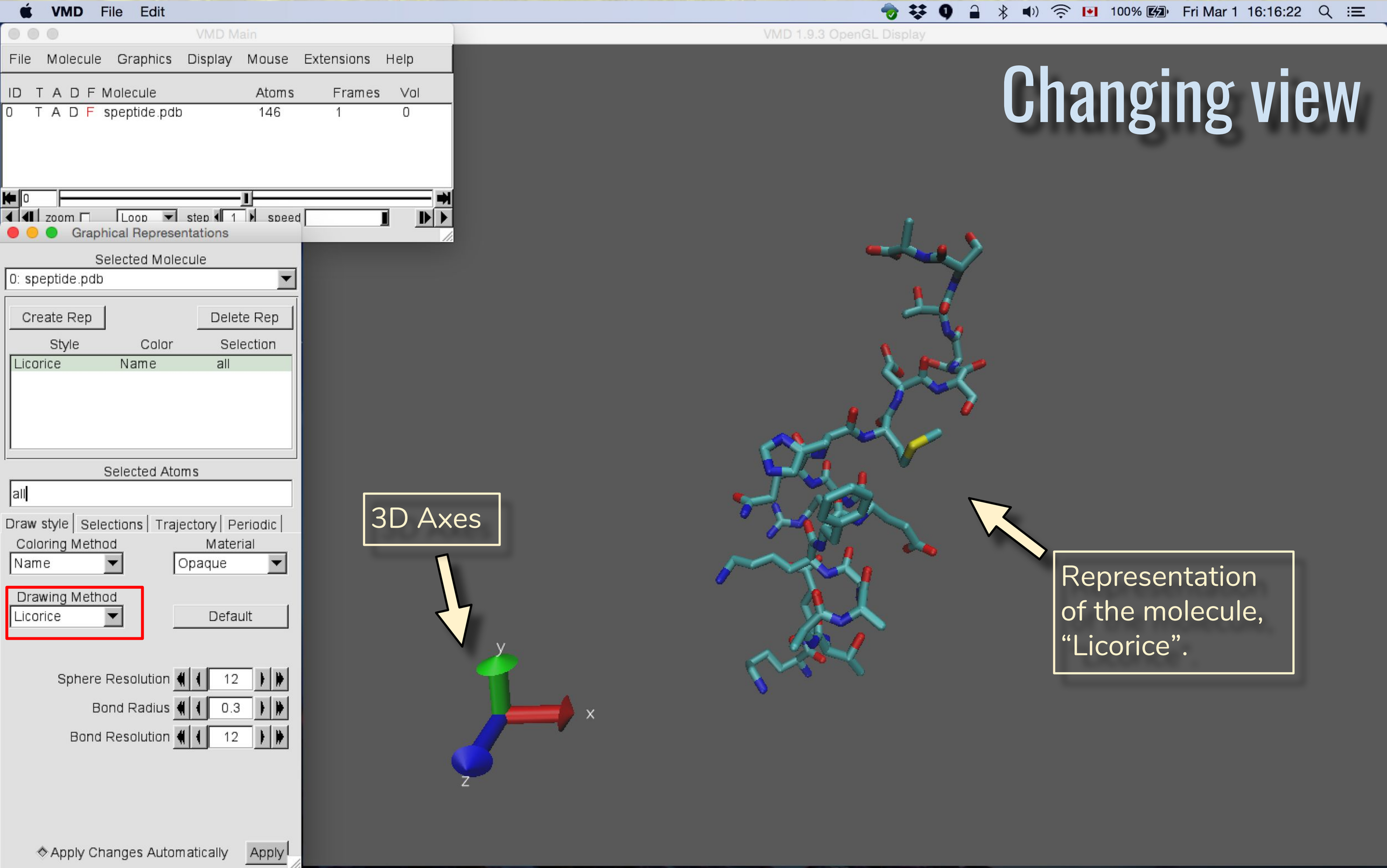
Categories

Colour Selector

Colour Editor



Changing view



VMD File Edit

100% Fri Mar 1 16:23:25

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

Sphere Resolution 12

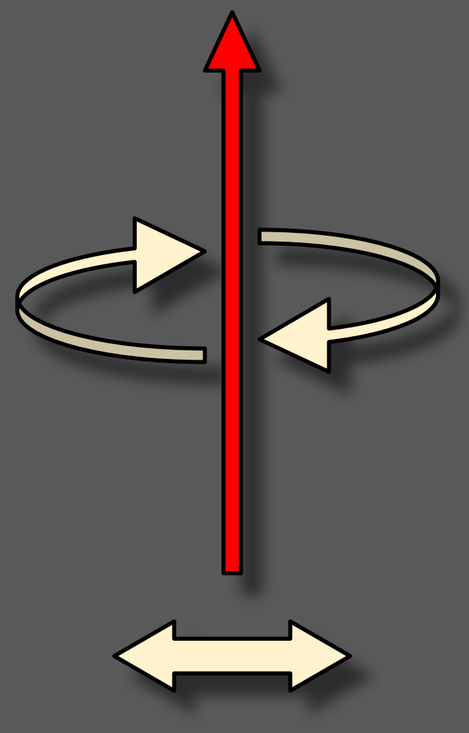
Bond Radius 0.3

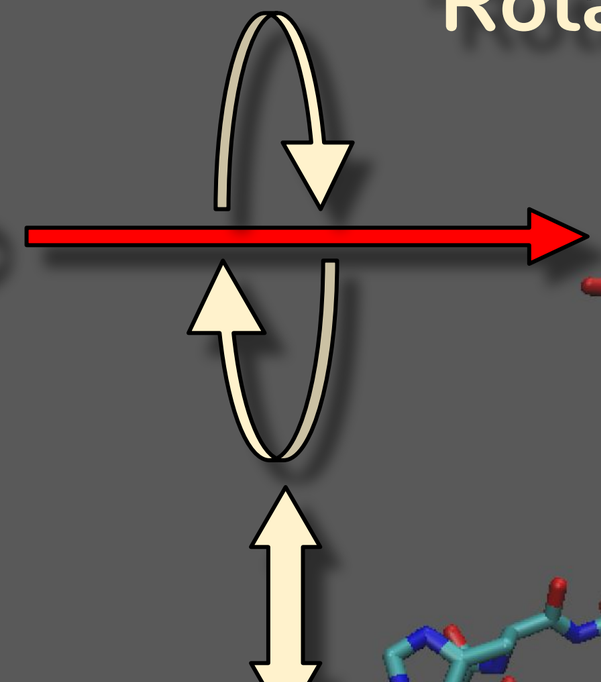
Bond Resolution 12

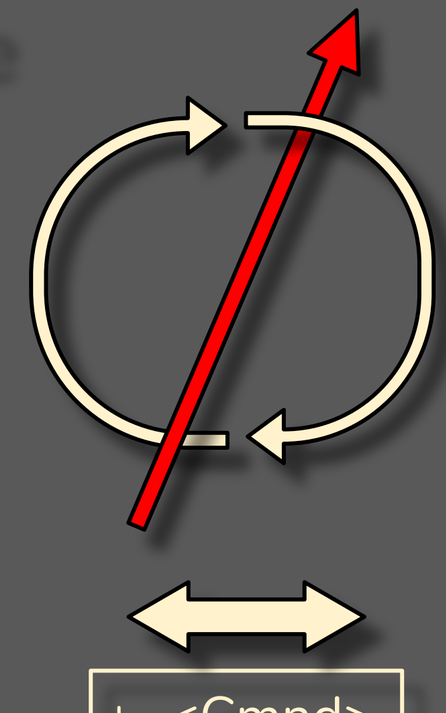
Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

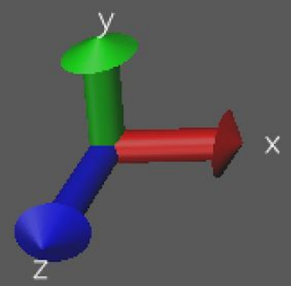
“Rotate” mode







+ <Cmnd>



Scrolling or Mouse wheel for **Zooming**

Changing view

VMD File Edit — 100% Fri Mar 1 16:54:31

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide.pdb

Create Rep | Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

Sphere Resolution 12

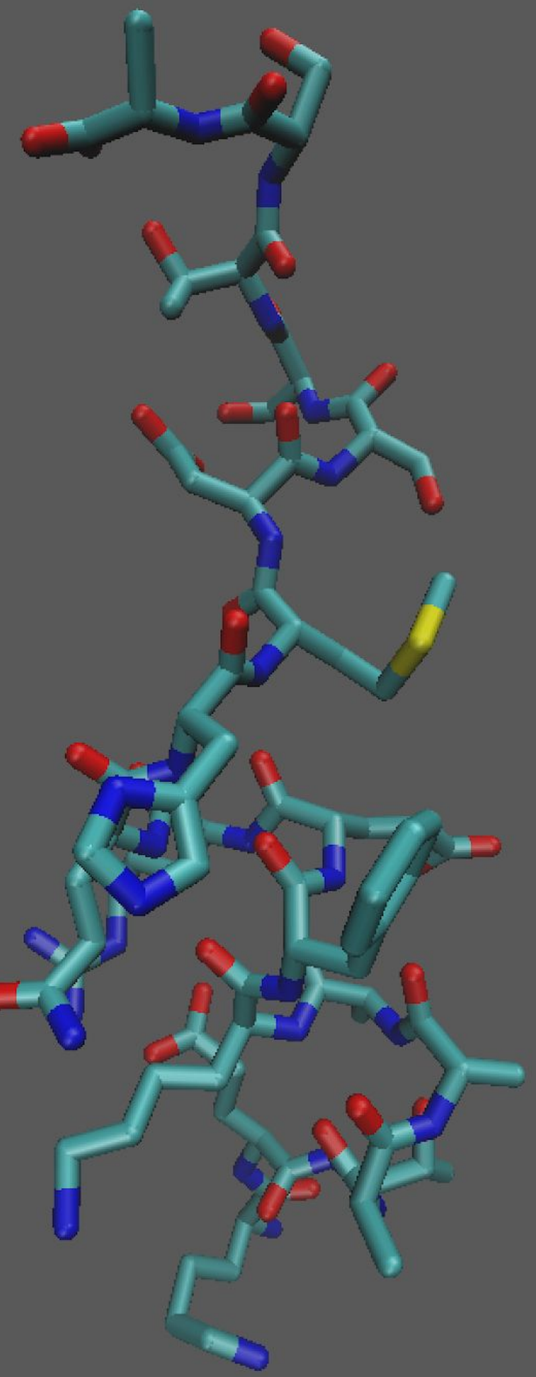
Bond Radius 0.3

Bond Resolution 12

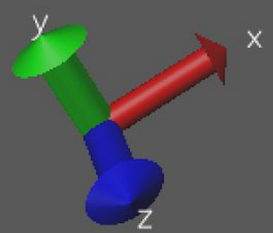
Apply Changes Automatically | Apply

VMD 1.9.3 OpenGL Display

"R" - rotate
"T" - translate
"S" - scale
"C" - center
"=" - reset view



- Rotate Mode R
- Translate Mode T
- Scale Mode S
- Center C
- Query 0
- Label
- Move
- Force
- Move Light
- Add/Remove Bonds
- Pick P



Changing view does not affect actual atomic positions. Only changes the view point.

Changing view

VMD File Edit

100% Sat Mar 2 14:32:05

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style	Color	Selection
VDW	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: VDW

Default

Sphere Scale 1.0

Sphere Resolution 12

Apply Changes Automatically Apply

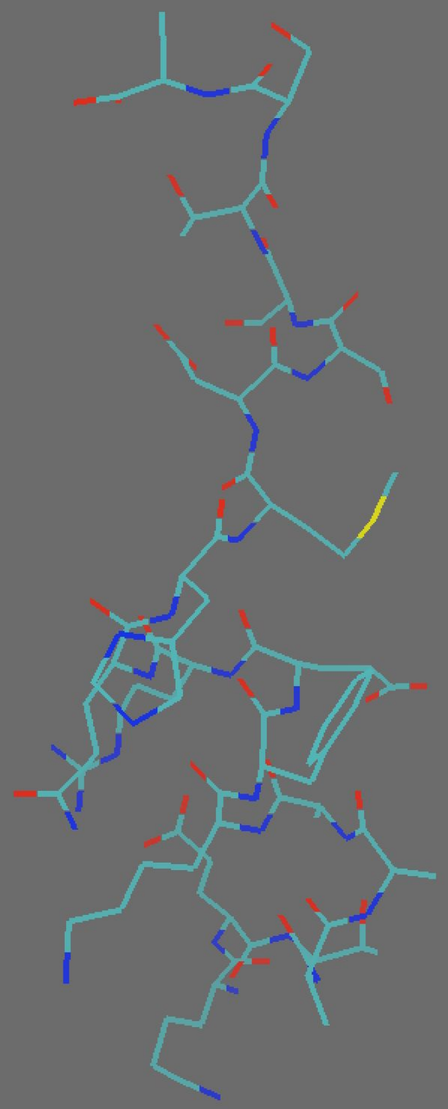
VMD 1.9.3 OpenGL Display

VDW:
Van-der-Waals spheres.
Roughly represent
Actual size of the atoms.

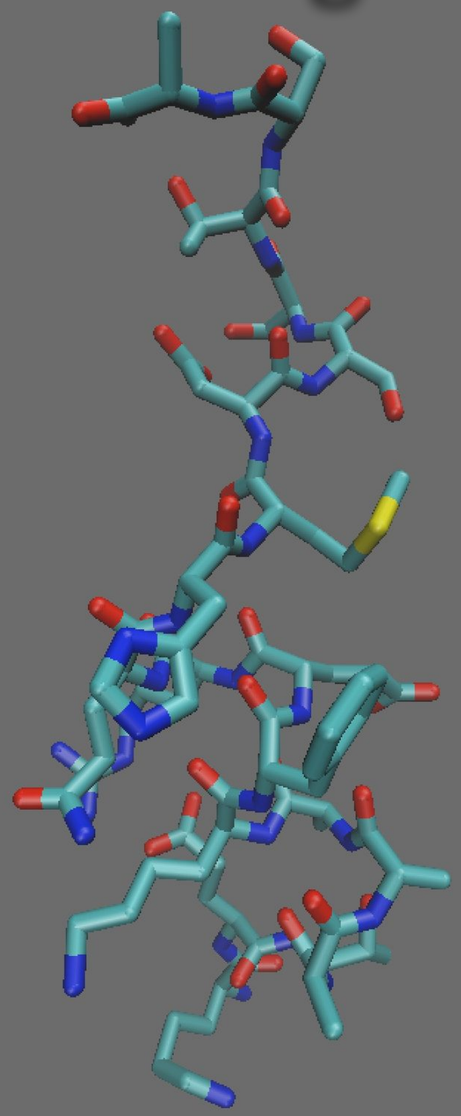
y x z

Drawing methods

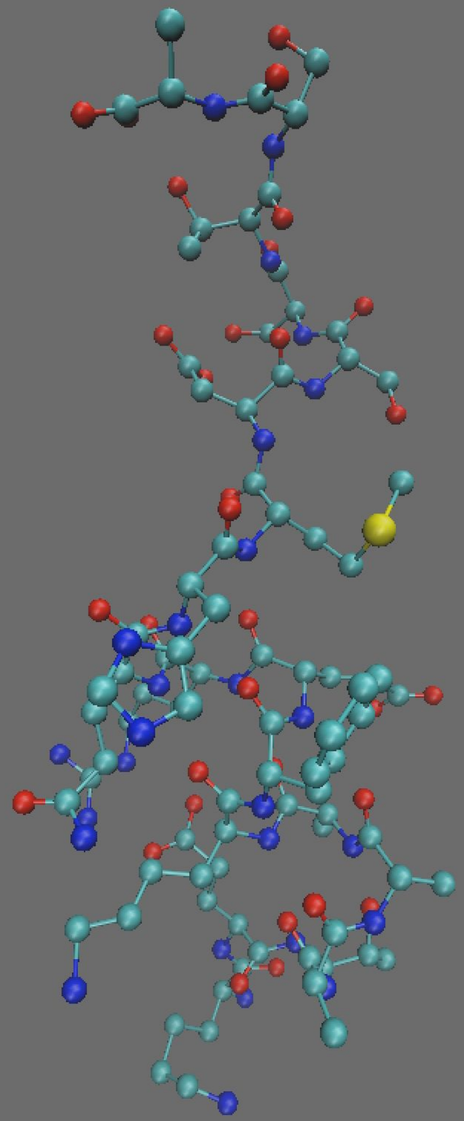
Atomistic Drawing Methods



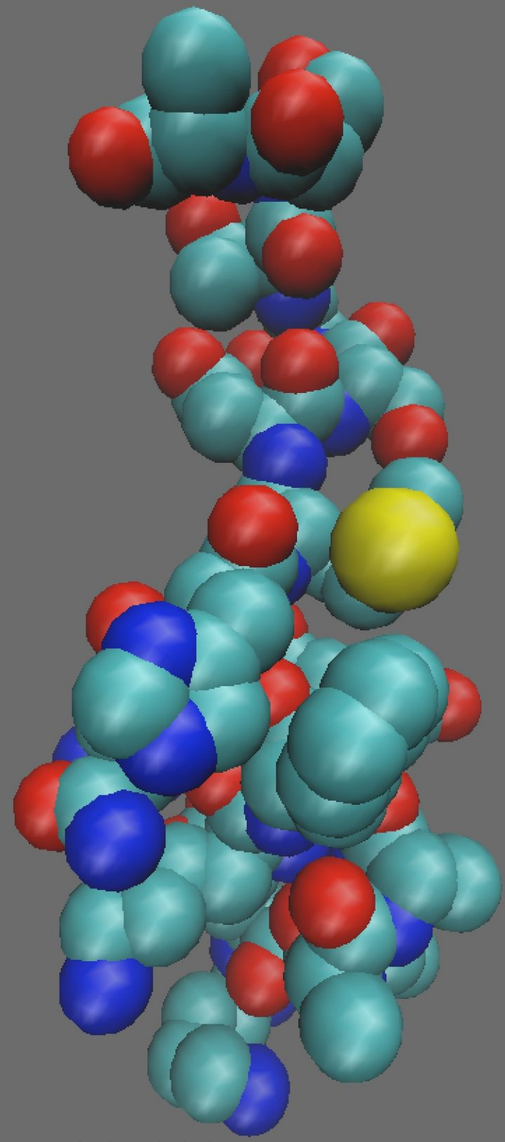
Lines:
Structure, atoms.
Very lightweight.
Default.



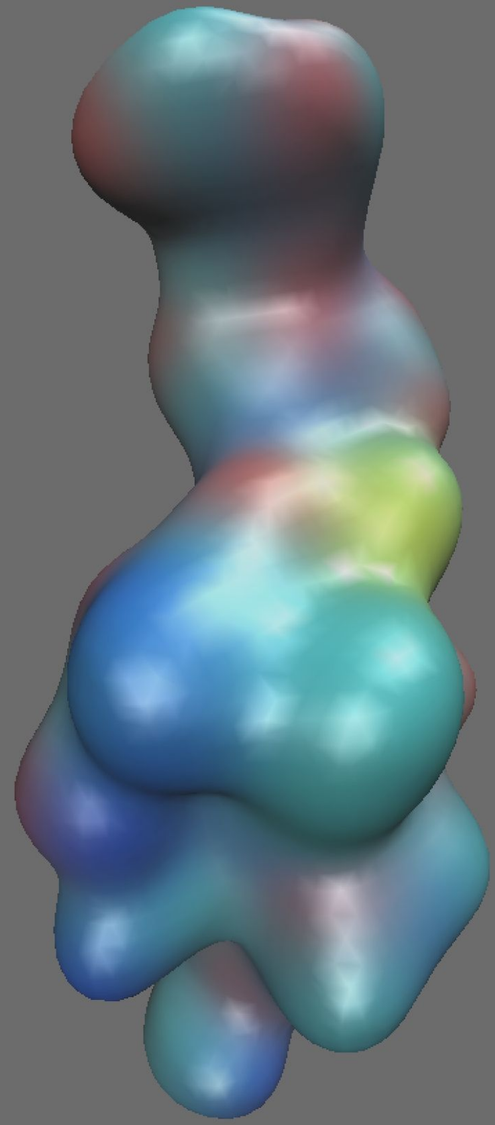
Licorice:
Structure, atoms.
Minimalistic.
Looks better.



CPK:
Structure, atoms.
Relative atom sizes.
Demanding.
Often too cluttered.



VDW:
Structure, atoms.
Realistic volume.
Too ugly.
Cluttered.



Quick Surf:
Volume.
Clean.

VMD File Edit

100% Sat Mar 2 16:00:19

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Secondary Stru

Material: Opaque

Drawing Method: NewCartoon

Default

Spline Style: Catmull-Rom

Aspect Ratio 4.10

Thickness 0.30

Resolution 10

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

Coil

Turn

Coil

NewCartoon:
Secondary structure
based method.
Highlights structural motifs.
Removes atomistic details.

Secondary Structure coloring.

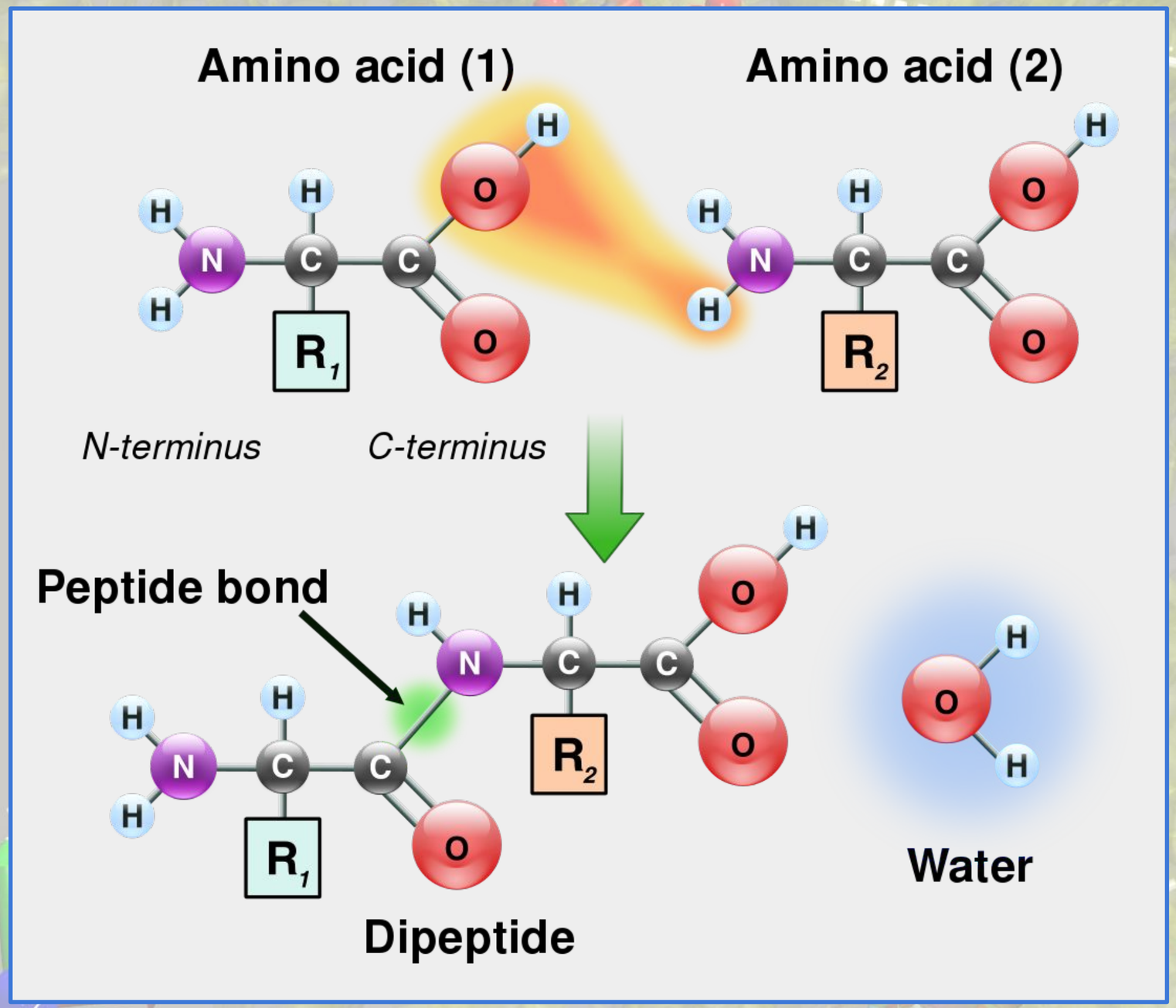
alpha-Helix

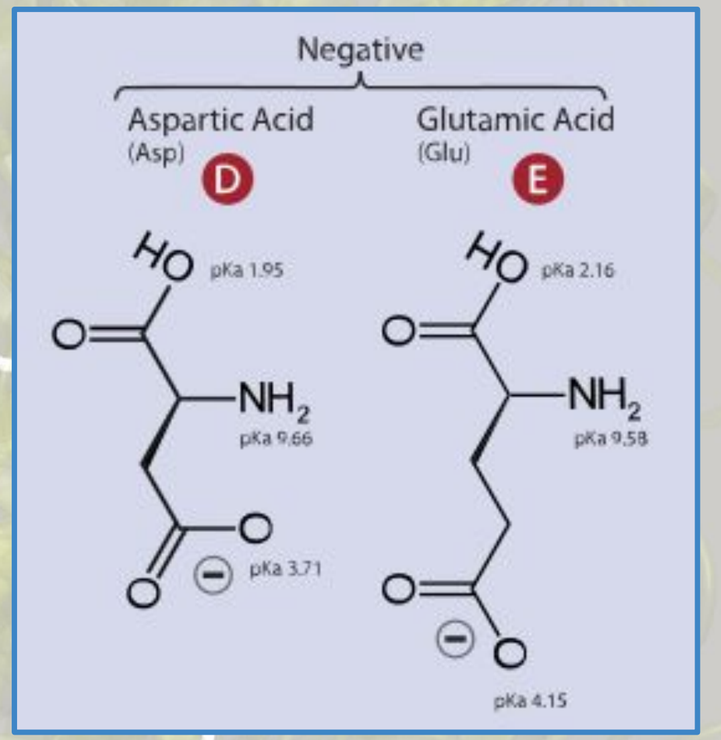
y x z

Coil

Drawing methods

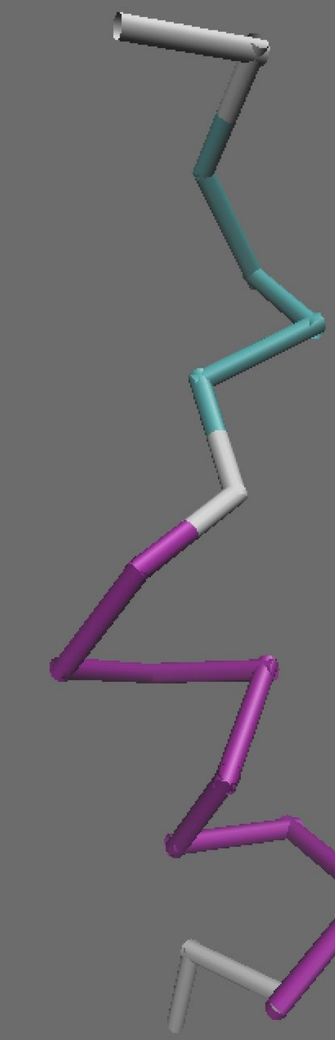
Peptide bonds and peptides





- **21 amino acids** for proteins;
- **Peptide**: **2 to 50** amino acids.
- **Protein**: **> 50** amino acids in the chain.
- Long chains form 3D motifs, called **secondary structure**.
- **Backbone**: $[C\text{-}C\text{-}N]_n$.
- Most common: **alpha-helices** and **beta-sheets**.

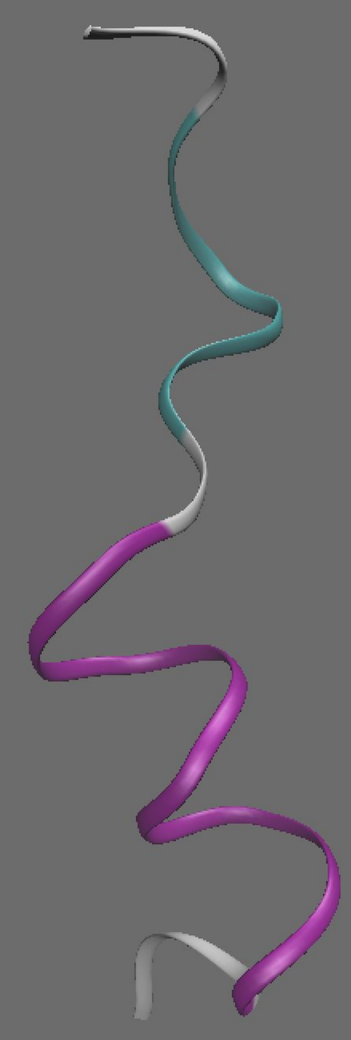
Secondary Structure based Drawing Methods



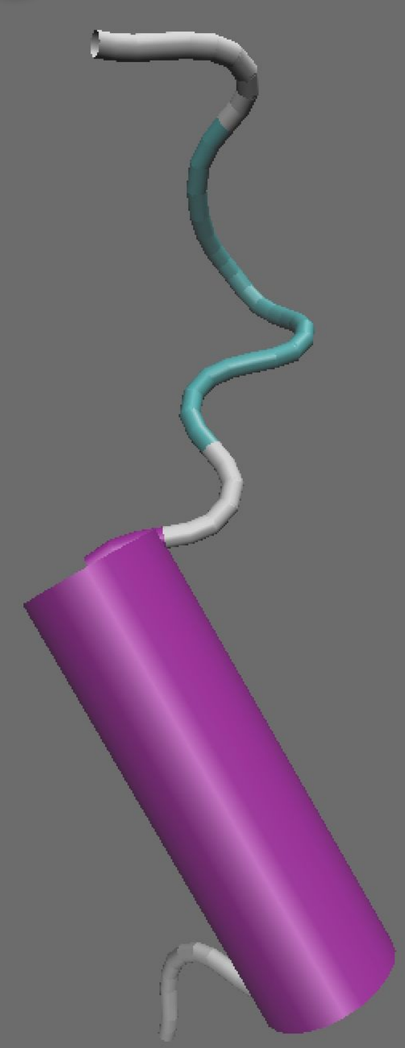
Trace:
Peptide backbone information.

Tube:
Smoothed backbone. Looks much cleaner.

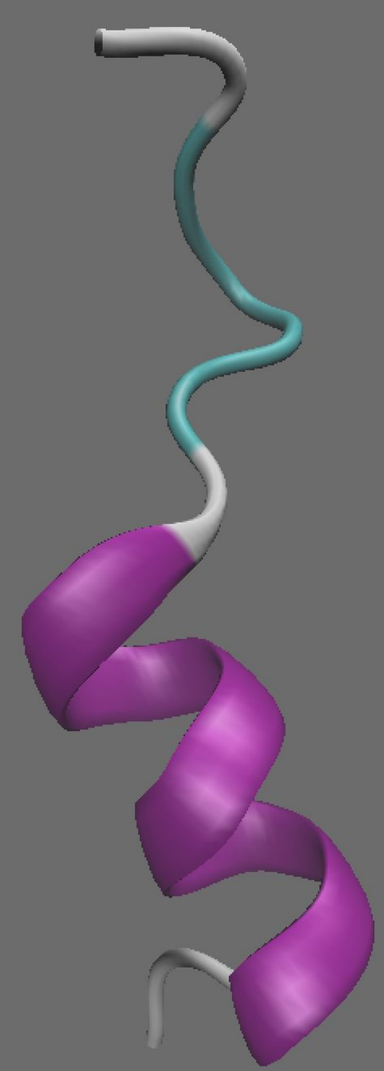
Ribbons:
Backbone orientation information



NewRibbons:
Cleaner new version.



Cartoon:
Backbone with Secondary motif assignments.



NewCartoon:
Cleaner new version.

VMD File Edit — 100% Sat Mar 2 17:16:04

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style	Color	Selection
VDW	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: VDW

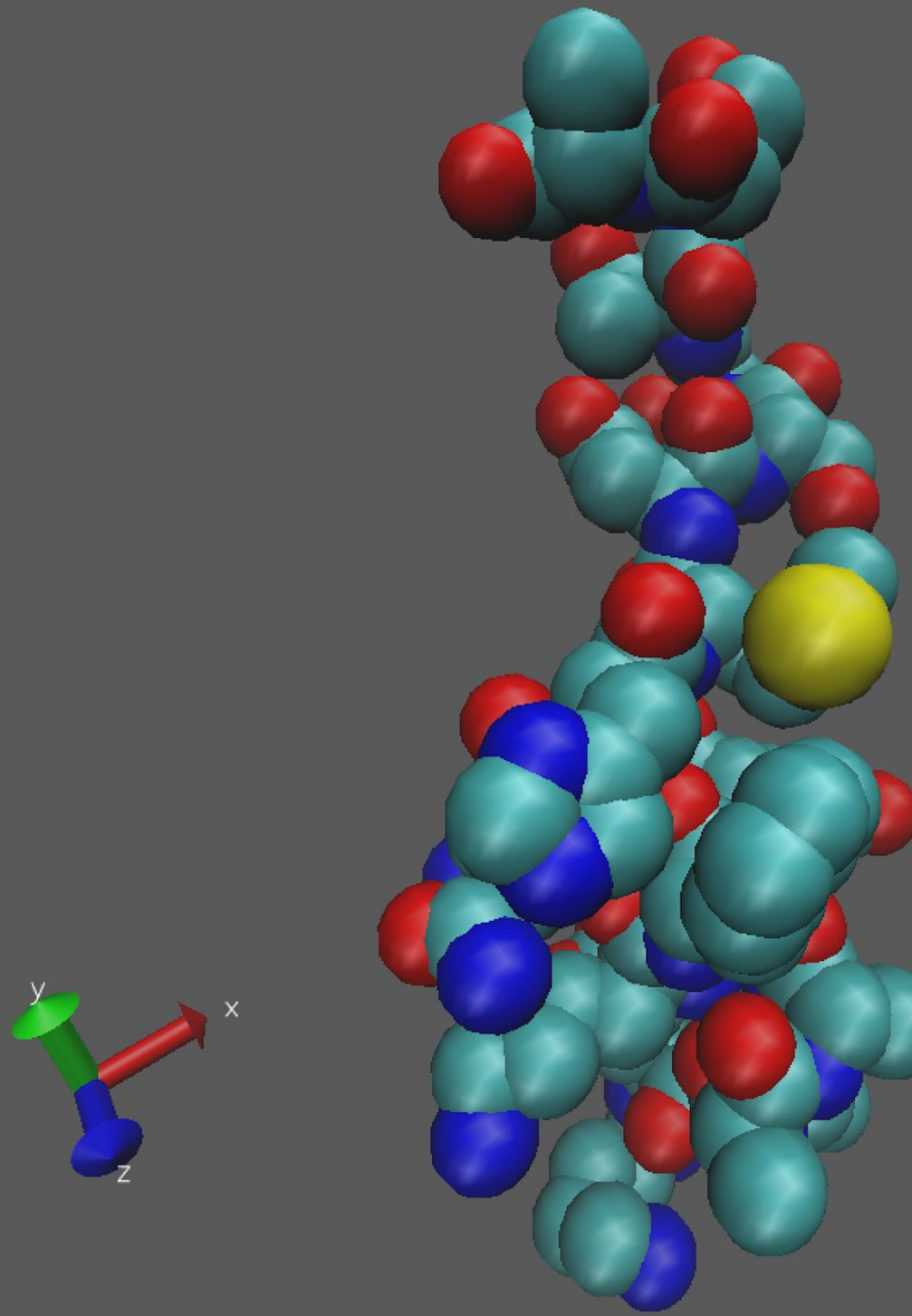
Default

Sphere Scale 1.0

Sphere Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display



VDW drawing method hides secondary structure well.

Note that atoms at farther distance look smaller.

It is due to **Perspective** screen projection mode.

Display modes

VMD File Edit — 100% Sat Mar 2 17:16:25

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID T A D F Molecule — Frames Vol

0 T A D F speptide.pdb — 1 0

Reset View
Stop Rotation
Perspective
Orthographic
Antialiasing
Depth Cueing
Culling
FPS Indicator
Light 0
Light 1
Light 2
Light 3
Axes
Background
Stage
Stereo
Stereo Eye Swap
Cachemode
Rendermode
Display Settings...

zoom Loop

Selected Mole

0: speptide.pdb

Create Rep

Style Color

VDW Name

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: VDW

Default

Sphere Scale 1.0

Sphere Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

y x z

Perspective:

- Adds 3D perspective;
- Looks better on illustrations.
- Distorts size perception.

Orthographic:

- Parallel projection;
- Same size at different distances.
- Better for structural analysis.

Screen Projection

VMD File Edit 100% Sat Mar 2 17:16:47

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Frames	Vol
0	T	A	D	F	speptide.pdb	1	0

Reset View
Stop Rotation
Perspective
Orthographic
Antialiasing
Depth Cueing
Culling
FPS Indicator
Light 0
Light 1
Light 2
Light 3
Axes
Background
Stage
Stereo
Stereo Eye Swap
Cachemode
Rendermode
Display Settings...

zoom Loop

Selected Mole
0: speptide.pdb

Create Rep
Style Color
VDW Name

Selected Atoms
all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name
Material: Opaque
Drawing Method: VDW
Default

Sphere Scale 1.0
Sphere Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

y
x
z

Depth Cueing:

- Improves 3D depth perception;
- Makes the model look dull.
- Could be useful for final rendering.

Depth Cueing

VMD File Edit — 100% Sat Mar 2 17:17:01

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Frames	Vol
0	T	A	D	F	speptide.pdb	1	0

Reset View
Stop Rotation
Perspective
Orthographic
Antialiasing
Depth Cueing
Culling
FPS Indicator
Light 0
Light 1
Light 2
Light 3
Axes
Background
Stage
Stereo
Stereo Eye Swap
Cachemode
Rendermode
Display Settings...

Rendermode: Normal, GLSL, Acrobat3D

zoom Loop

Selected Mole
0: speptide.pdb

Create Rep
Style Color
VDW Name

Selected Atoms
all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name
Material: Opaque
Drawing Method: VDW
Default

Sphere Scale 1.0
Sphere Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

y x z

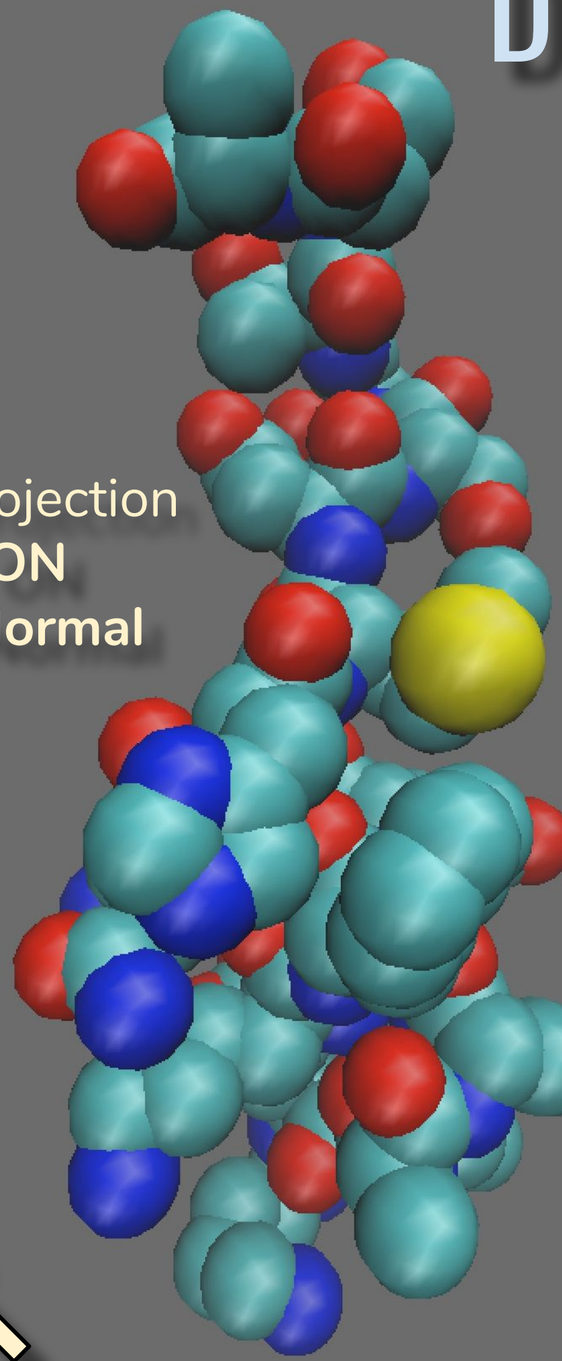
Rendermode GLSL:
Hardware accelerated mode.

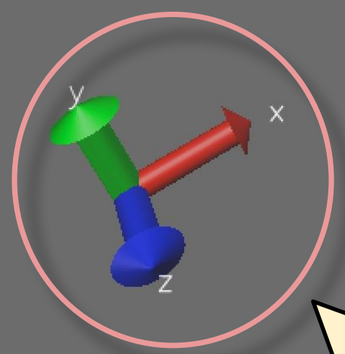
- Faster;
- Better looking;
- Needs a GPU video card.
- Much better for transparent materials.

Rendermode

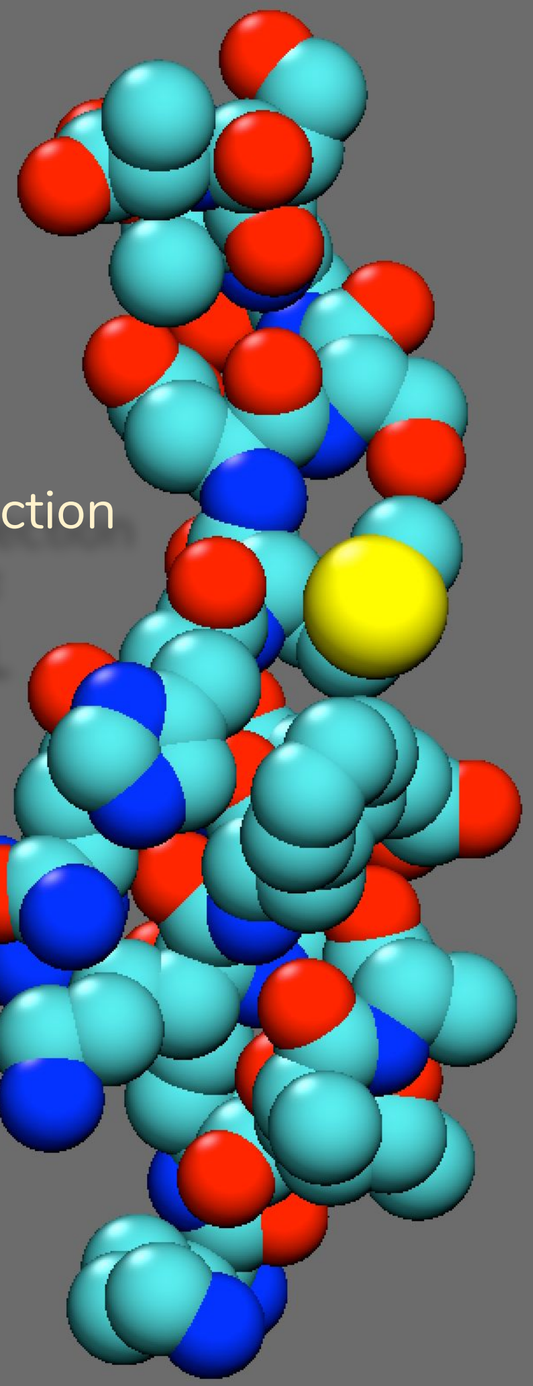
Display modes

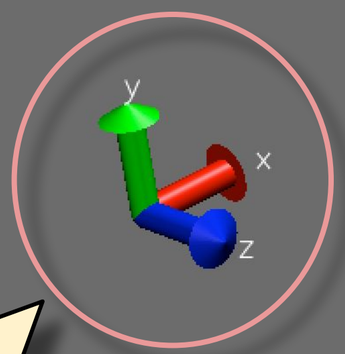
- **Perspective** projection
- Depth Cueing **ON**
- Rendermode **Normal**





- **Orthographic** projection
- Depth Cueing **OFF**
- Rendermode **GLSL**





Same point of view, but axes look very different.

Test case: Creating an illustration

- Create a publication quality illustration for the “**speptide**” molecule.
- Demonstrate the **structure** of the molecule.
- Indicate the presence of the **secondary structure** motifs in the peptide chain.
- Show the connection between the **primary** and **secondary** structures representation.
- Demonstrate realistic **volume** of the molecule.
- Provide information about actual **size** of the molecule.

VMD File Edit

100% Sun Mar 3 15:06:21

VMD Main

VMD 1.9.3 OpenGL Display

File Molecule Graphics Display Mouse Extensions Help

ID T A D F Molecule Frames Vol

0 T A D F speptide.pdb 1 0

zoom Loop

Selected Mole

0: speptide.pdb

Create Rep

Style Color

Lines Name

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method

Name

Material

Opaque

Drawing Method

Lines

Default

Thickness 4

Apply Changes Automatically Apply

Reset View

Stop Rotation

Perspective

Orthographic

Antialiasing

Depth Cueing

Culling

FPS Indicator

Light 0

Light 1

Light 2

Light 3

Axes

Background

Stage

Stereo

Stereo Eye Swap

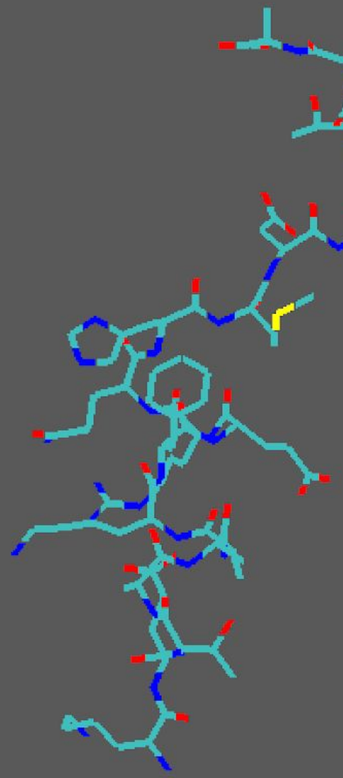
Cachemode

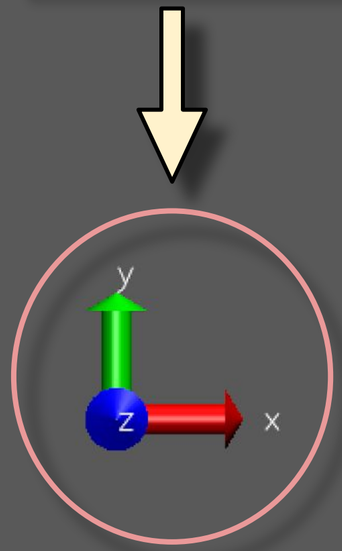
Rendermode

Display Settings...

1. Reset View
2. Drawing method: **Lines**
3. Thickness: 4

Note the new orientation.





Working on an illustration

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0		A	D	F	speptide.pdb	146	1	0
1		A	D	F	speptide.pdb	146	1	0
2	T	A	D	F	speptide.pdb	146	1	0

0 zoom Loop step 1 speed

Selected Molecule

2: speptide.pdb

Create Rep Delete Rep

Style Color Selection

Lines Name all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

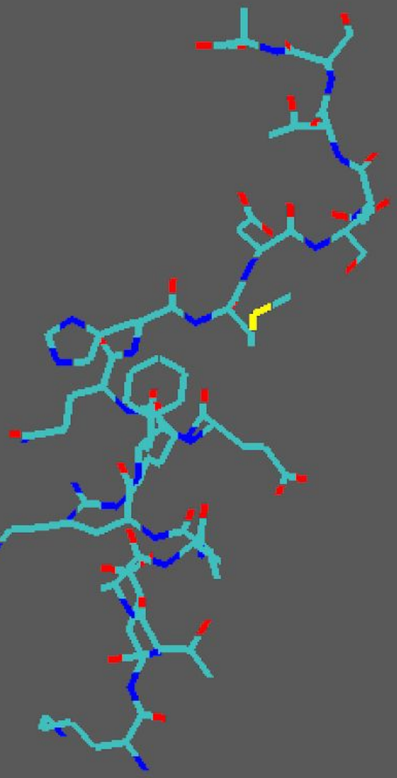
Default

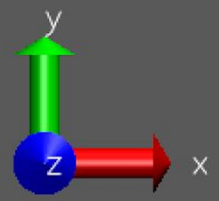
Thickness 1

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

- Load the same molecule two more times, so that three copies of the molecule are loaded.





Working on an illustration

VMD File Edit

100% Sun Mar 3 15:10:25

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0		A	D	F	speptide.pdb	146	1	0
1		A	D	F	speptide.pdb	146	1	0
2	T	A	D	F	speptide.pdb	146	1	0

0

zoom Loop

Selected M

2: speptide.pdb

Create Rep Delete Rep

Style Color Selection

Lines Name all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Default

Thickness 1

Apply Changes Automatically Apply

?

Enter a new name for molecule 0:

speptide structure

OK Cancel

VMD 1.9.3 OpenGL Display

y

z x

- Rename the copies to make them distinguishable.
- Double click on the molecule name to bring up the dialog.

Working on an illustration

VMD File Edit — 100% Sun Mar 3 15:10:51

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0		A	D	F	speptide structure	146	1	0
1		A	D	F	speptide cartoon	146	1	0
2	T	A	D	F	speptide volume	146	1	0

0 zoom Loop step 1 speed

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style Color Selection

Lines Name all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

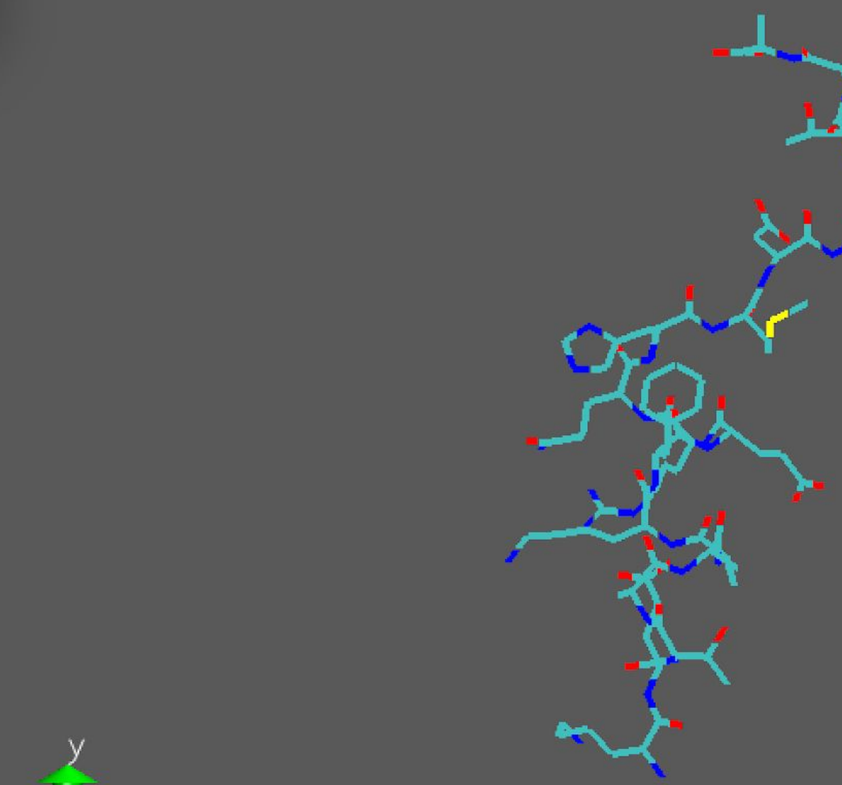
Default

Thickness 1

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

1. speptide structure;
2. speptide cartoon;
3. speptide volume;



Working on an illustration

VMD File Edit — 100% Sun Mar 3 15:11:39

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0		A	D	F	speptide structure	146	1	0
1		A	D	F	speptide cartoon	146	1	0
2	T	A	D	F	speptide volume	146	1	0

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide structure

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

Sphere Resolution 12

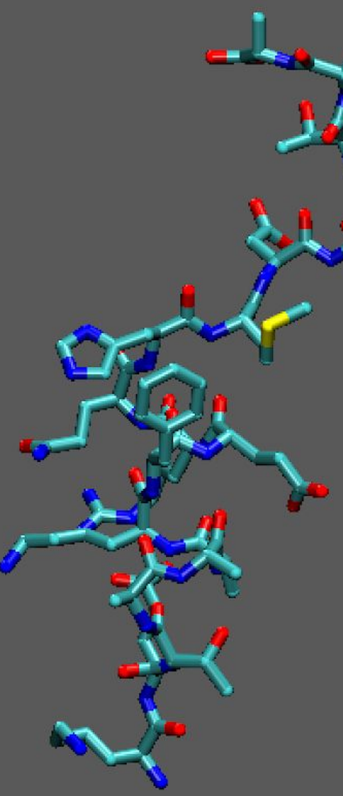
Bond Radius 0.3

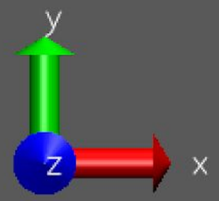
Bond Resolution 12

Apply Changes Automatically Apply

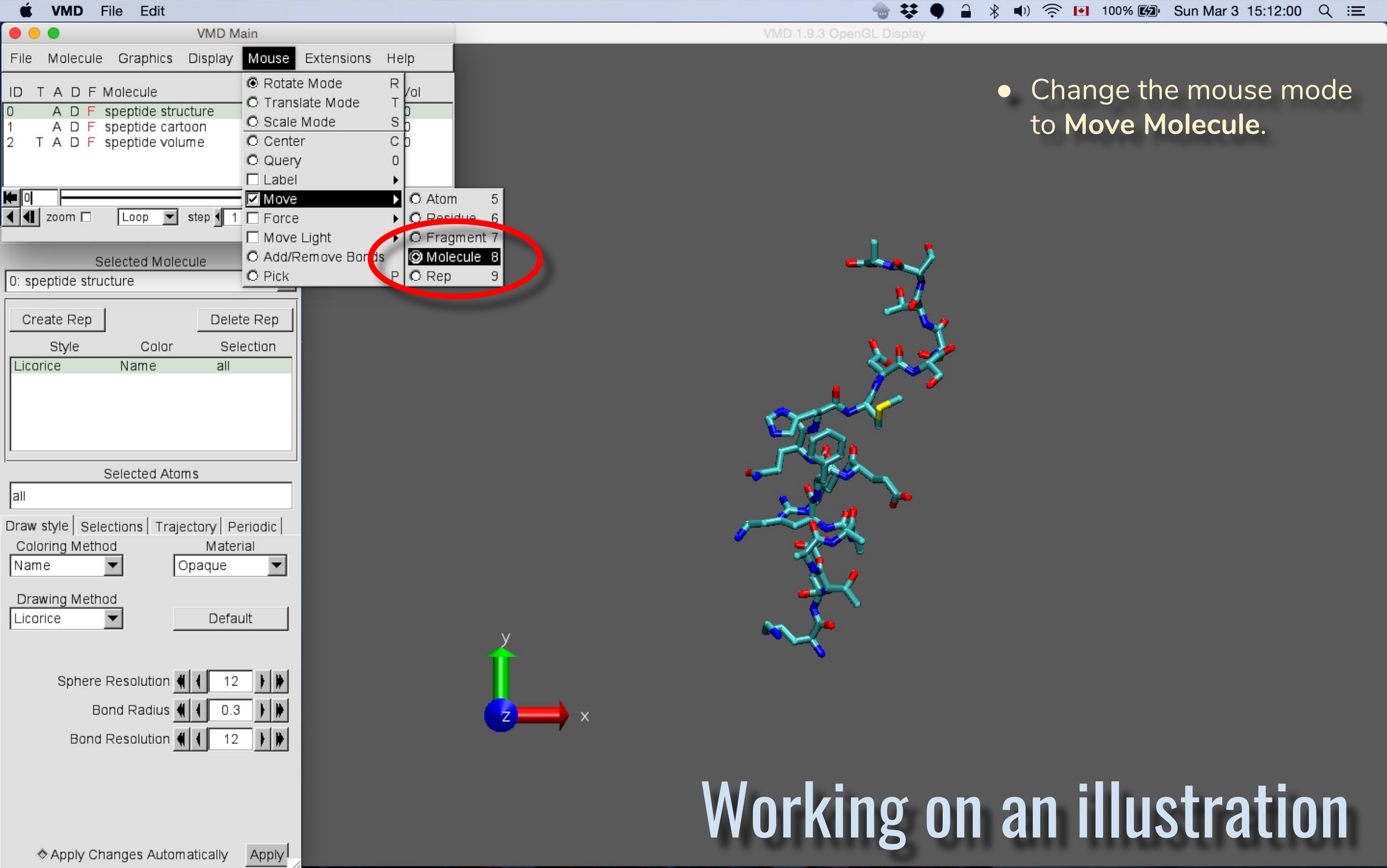
VMD 1.9.3 OpenGL Display

- Change the **representation** of the first molecule to **licorice** to make it easier to pick up with the pointer.





Working on an illustration


VMD File Edit
100% Sun Mar 3 15:12:00
VMD Main
VMD 1.9.3 OpenGL Display
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule
0 A D F speptide structure
1 A D F speptide cartoon
2 T A D F speptide volume
Rotate Mode R
Translate Mode T
Scale Mode S
Center C
Query 0
Label
Move
Force
Move Light
Add/Remove Bonds
Pick P
Atom 5
Residue 6
Fragment 7
Molecule 8
Rep 9
zoom
Loop
step
Selected Molecule
0: speptide structure
Create Rep
Delete Rep
Style Color Selection
Licorice Name all
Selected Atoms
all
Draw style
Selections
Trajectory
Periodic
Coloring Method
Name
Material
Opaque
Drawing Method
Licorice
Default
Sphere Resolution 12
Bond Radius 0.3
Bond Resolution 12
Apply Changes Automatically
Apply
y
z
x
Change the mouse mode to Move Molecule.
Working on an illustration

VMD File Edit

100% Sun Mar 3 15:12:37

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0 zoom Loop step 1 speed

Selected Molecule

0: speptide structure

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

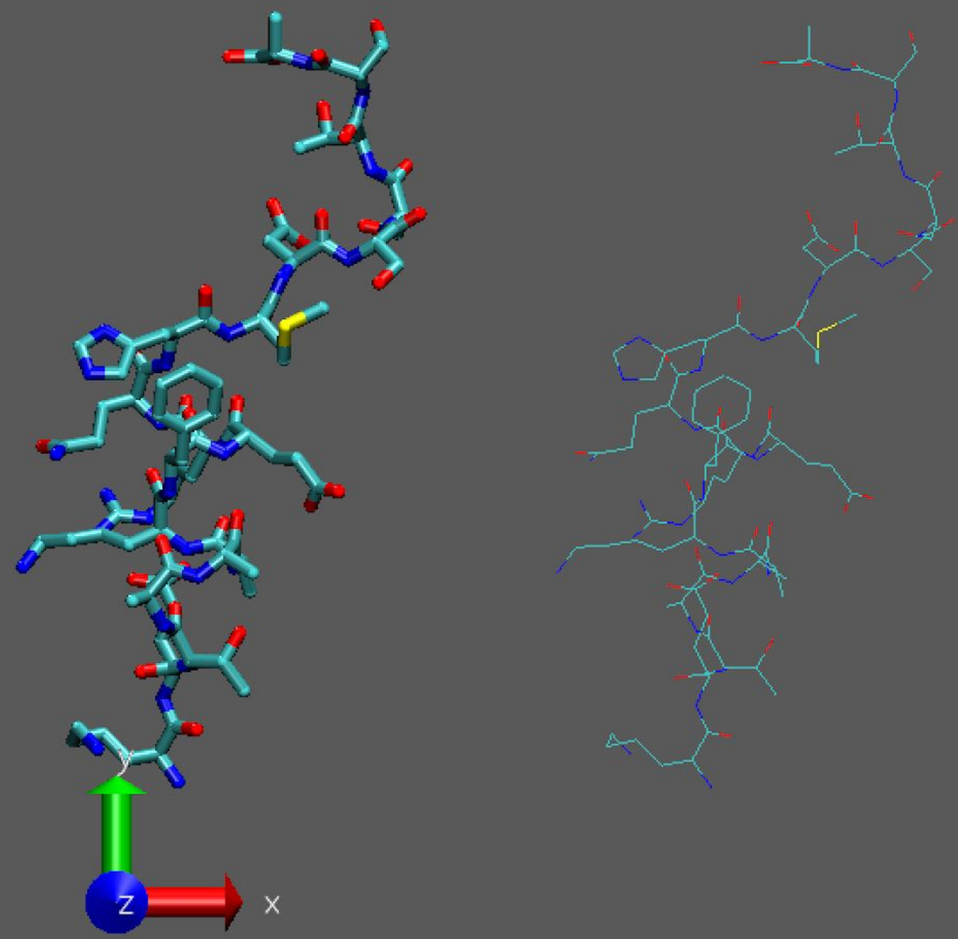
Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display



- Move the first **“structure”** molecule to the **left** part of the window.

Working on an illustration

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style Color Selection

Licorice Name all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

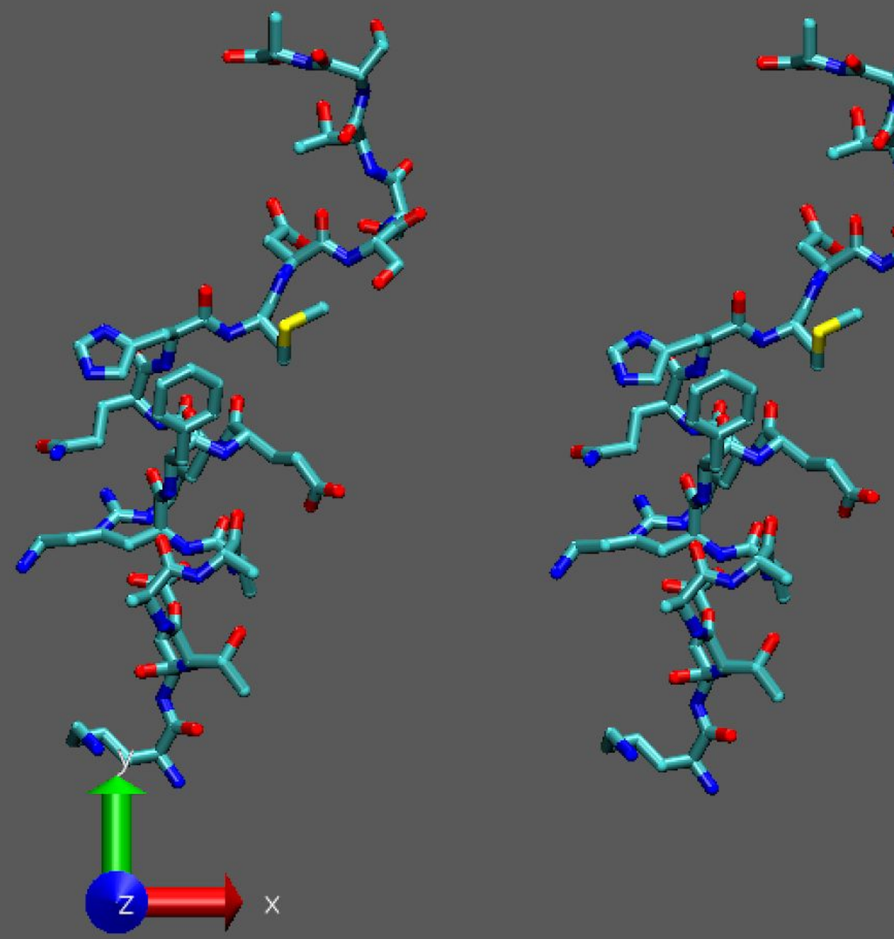
Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display



- Repeat with the "**volume**" molecule.

Working on an illustration

VMD File Edit — 100% Sun Mar 3 15:13:40

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

- Move to “**volume**” molecule to the right part of the window.

Z X

Working on an illustration

VMD File Edit

100% Sun Mar 3 15:16:10

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule
0		A	D	F	speptide structure
1		A	D	F	speptide cartoon
2	T	A	D	F	speptide volume

Rotate Mode R
Translate Mode T
Scale Mode S
Center C
Query 0
Label
Move
Force
Move Light
Add/Remove Bonds
Pick P

0 zoom Loop step 1

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Default

Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

- Change the mouse mode to “**Translate**”.

y
z
x

Working on an illustration

VMD File Edit — 100% Sun Mar 3 15:17:28

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

1: speptide cartoon

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Secondary Stru

Material: Opaque

Drawing Method: NewCartoon

Default

Spline Style: Catmull-Rom

Aspect Ratio 4.10

Thickness 0.30

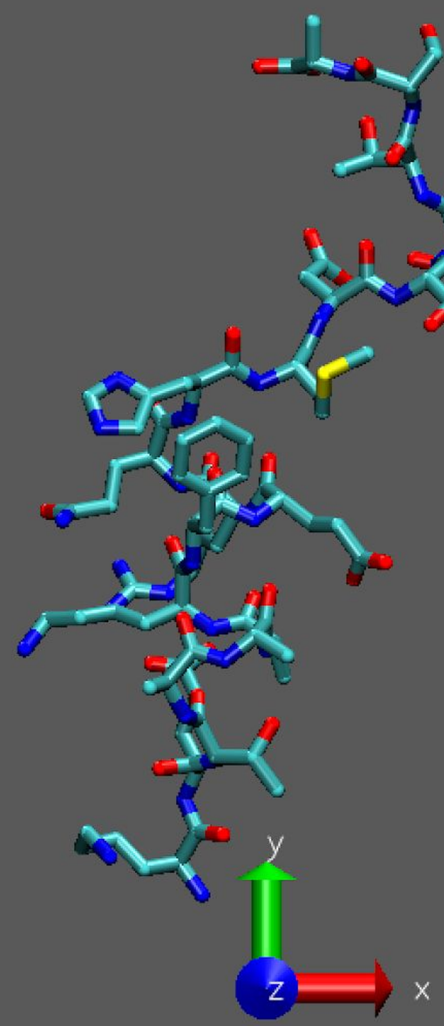
Resolution 10

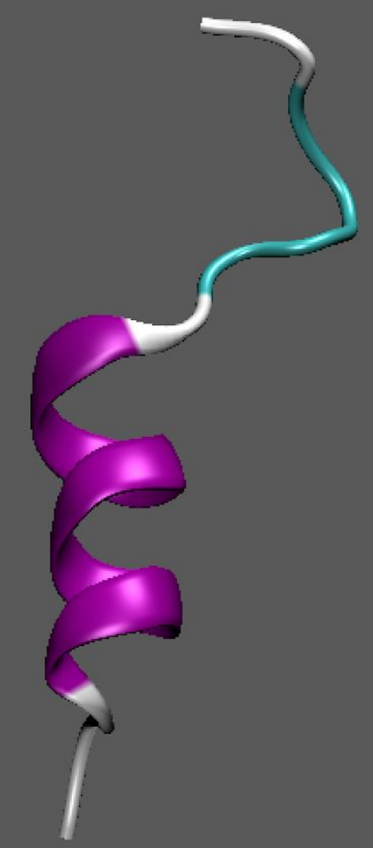
Apply Changes Automatically Apply

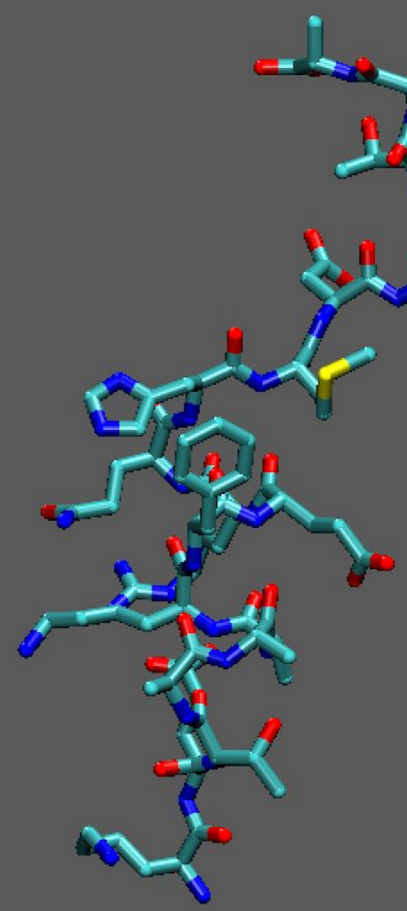
VMD 1.9.3 OpenGL Display

In **Representations** window:

- Select the "**cartoon**" molecule;
- Drawing method: **NewCartoon**;
- Coloring: **Secondary Structure**.

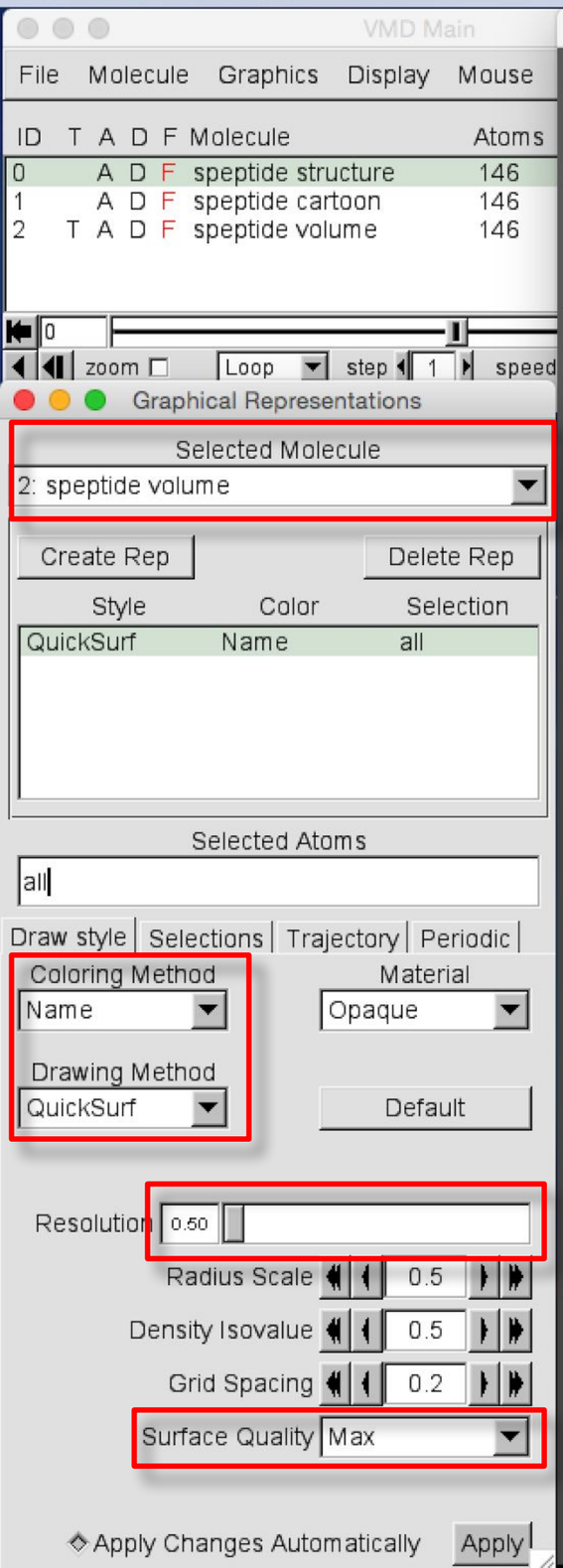


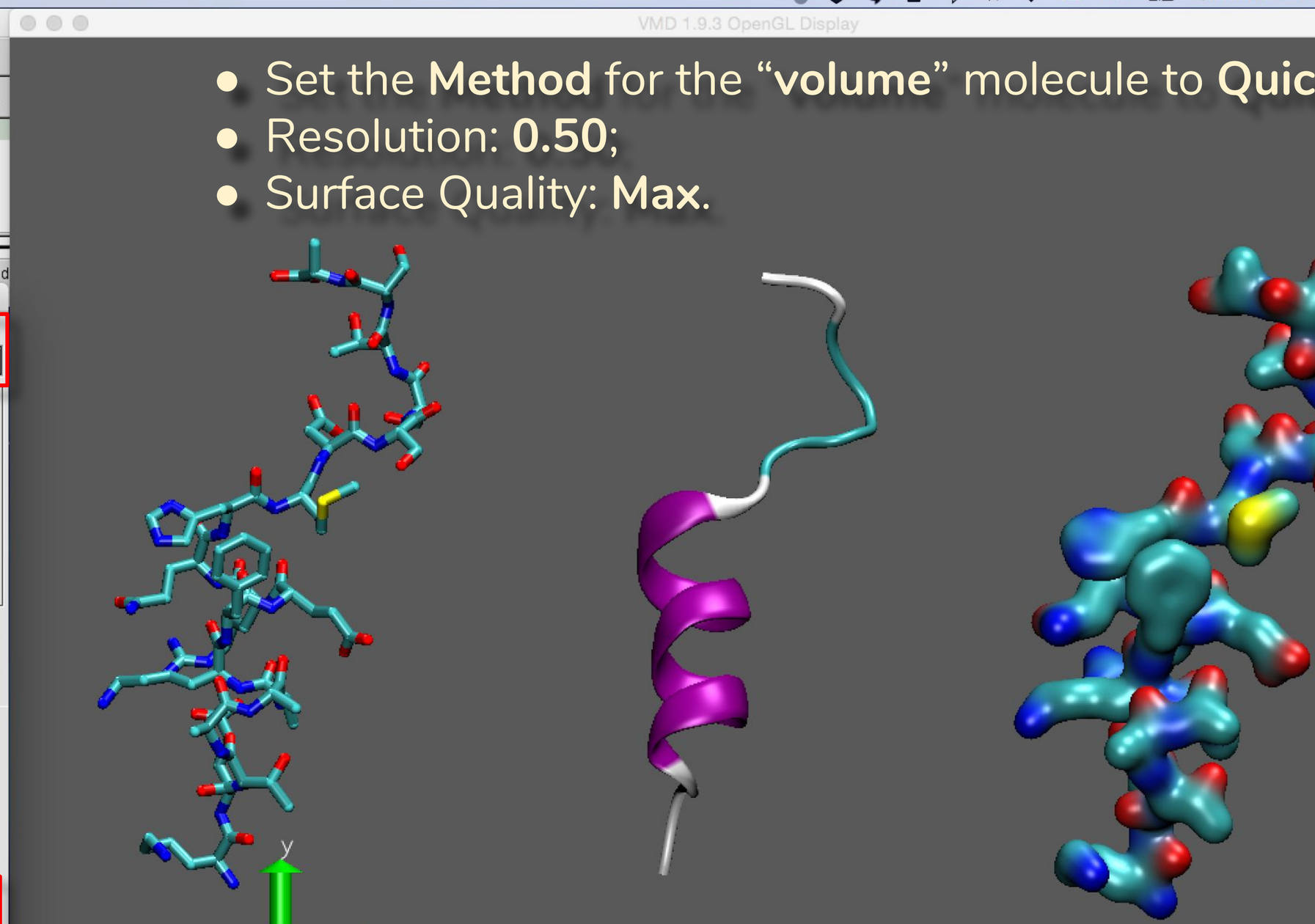




Working on an illustration

- Set the **Method** for the “**volume**” molecule to **QuickSurf**;
- Resolution: **0.50**;
- Surface Quality: **Max**.





Note that **QuickSurf** representation cannot be picked up in the **Move** mode. A helper VDW representation can be added for this purpose.

Working on an illustration

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Frames	Vol
0		A	D	F	speptide stru	1	0
1		A	D	F	speptide cart	1	0
2	T	A	D	F	speptide volu	1	0

0 zoom Loop

Selected Mole

2: speptide volume

Create Rep

Style Color

QuickSurf Name

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Opaque

Drawing Method: QuickSurf

Default

Resolution 0.50

Radius Scale 0.5

Density Isovalue 0.5

Grid Spacing 0.2

Surface Quality Max

Apply Changes Automatically Apply

Reset View

Stop Rotation

Perspective

Orthographic

Antialiasing

Depth Cueing

Culling

FPS Indicator

Light 0

Light 1

Light 2

Light 3

Axes

Background

Stage

Stereo

Stereo Eye Swap

Cachemode

Rendermode

Display Settings...

Off

Origin

LowerRight

UpperLeft

UpperRight

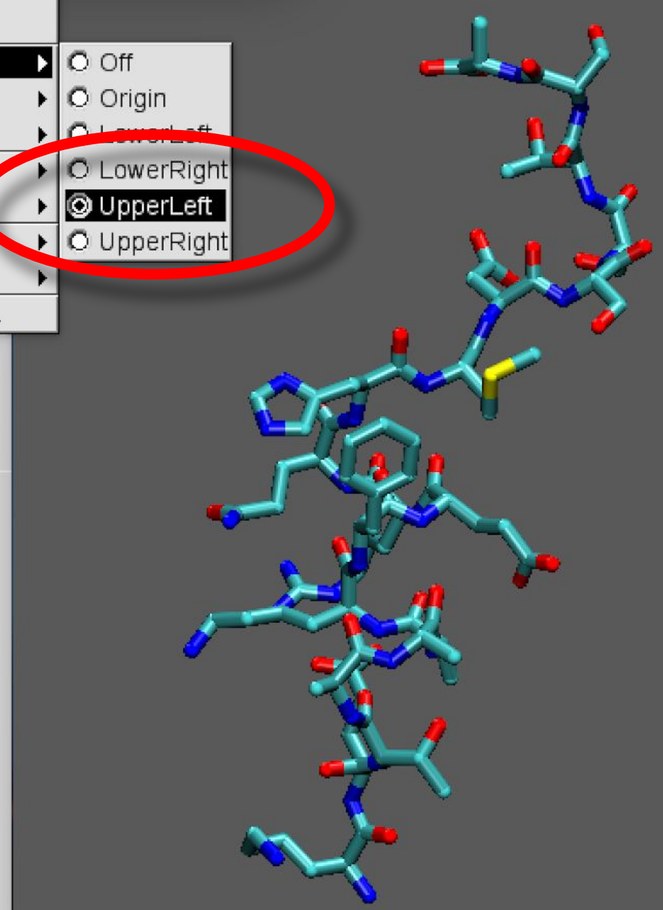
VMD 1.9.3 OpenGL Display

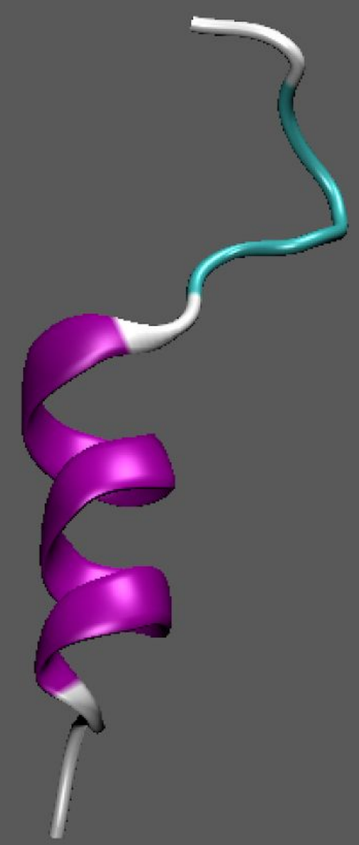
y

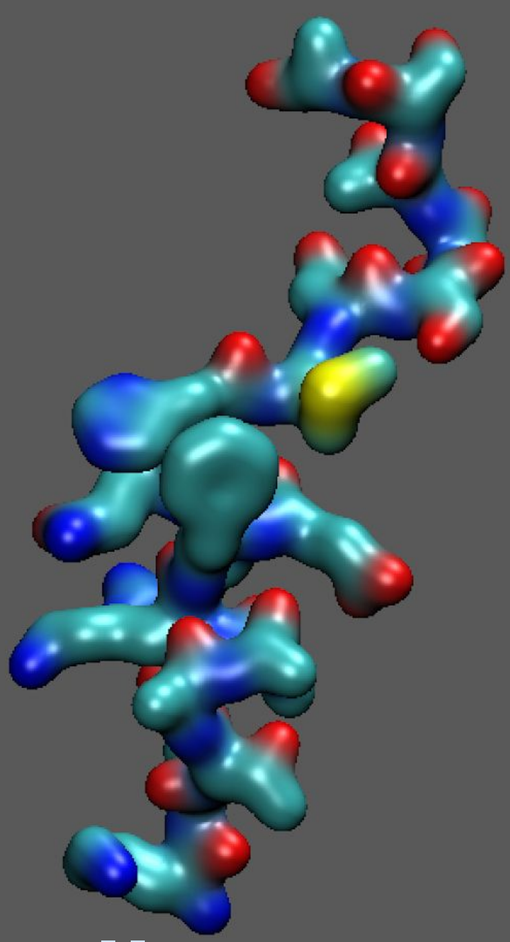
z

x

- Rearrange the work to have more space in the lower part of the window.
- Move the "**Axes**" to the **UpperLeft**.







Working on an illustration

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide structure

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all
Licorice	ColorID 3	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: ColorID 3

Material: Opaque

Drawing Method: Licorice

Default

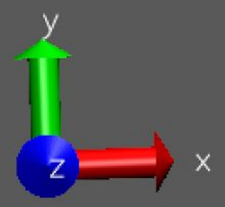
Sphere Resolution 12

Bond Radius 0.3

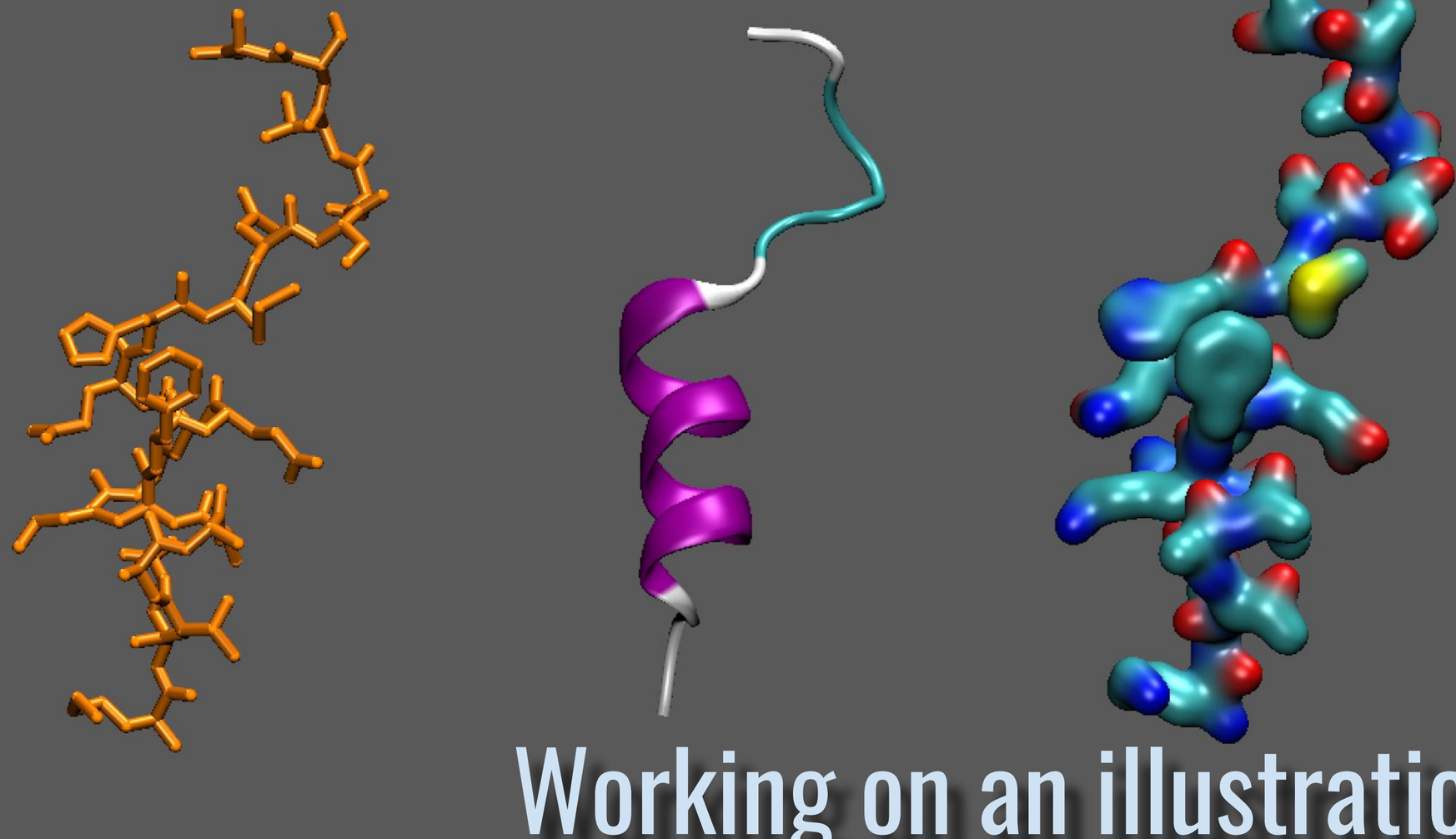
Bond Resolution 12

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display



- Select the “**structure**” molecule;
- **Create** new representation;
- Drawing method: **Licorice**;
- Coloring: **ColorID**;
- Color: **3** (Orange).



Working on an illustration

VMD File Edit

100% Sun Mar 3 15:23:04

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

0: speptide structure

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all
Licorice	ColorID 3	backbone

Selected Atoms

backbone

Draw style | Selections | Trajectory | Periodic

Singlewords

helix
alpha_helix
helix_3_10
pi_helix
sheet

and or not

Apply

Reset

Macro definition:

alpha_helix

Keyword	Value
charge	C
beta	H
occupancy	T
volindex0	
volindex1	
volindex2	
volindex3	
volindex4	
volindex5	

VMD 1.9.3 OpenGL Display

y x z

- For the **new representation**;
- Switch the Tab from **Draw style** to **Selections**.
- Set **Selected Atoms** to **backbone**.

Working on an illustration

VMD File Edit

100% Sun Mar 3 15:25:30

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

1: speptide cartoon

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all
VDW	Name	(name "N.*"

Selected Atoms

(name "N.*" "O.*" "S.*") and (not backbone)

Draw style | Selections | Trajectory | Periodic

Singlewords

helix
alpha_helix
helix_3_10
pi_helix
sheet

and or not

Apply

Reset

Macro definition:

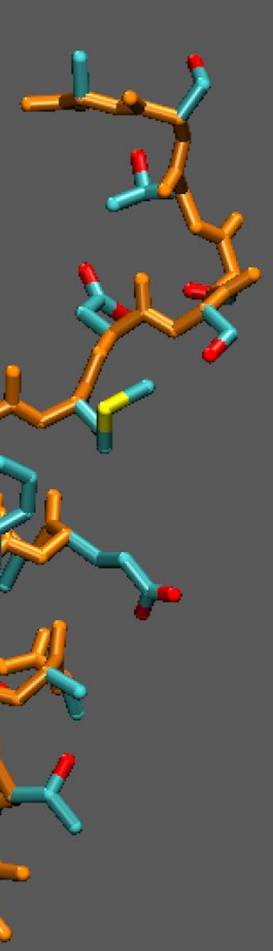
alpha_helix

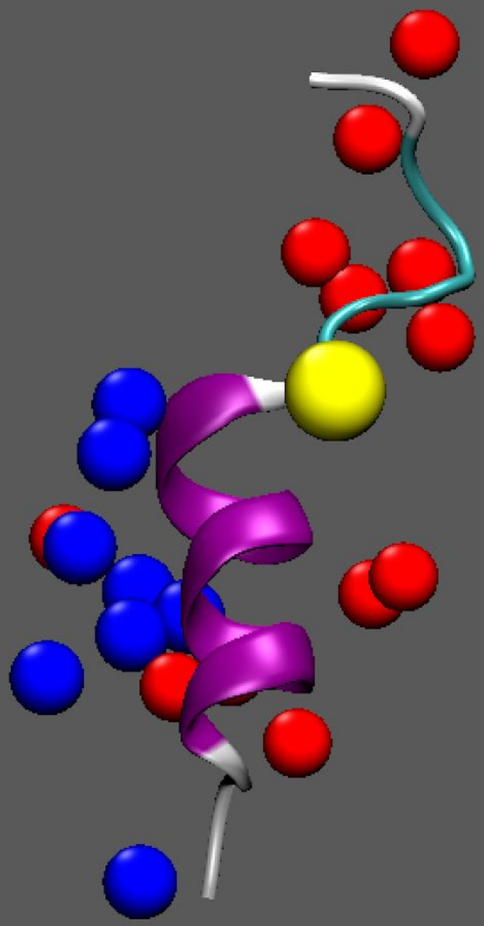
Keyword	Value
name	NZ
type	O
backbonetype	OD1
residuetype	OD2
index	OE1
serial	OE2
atomicnumber	OG
element	OG1
residue	SD

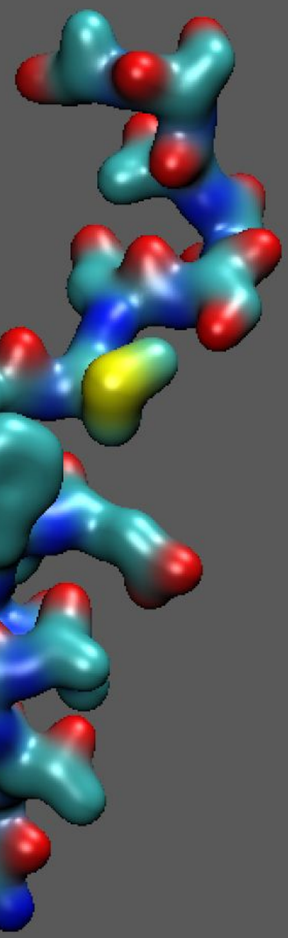
VMD 1.9.3 OpenGL Display

y x z

- Show **heteroatoms** in the "**cartoon**" molecule;
- **New** representation: **VDW** colored by **Name**;
- Switch to **Selections** Tab;
- **Selected Atoms**:
  (name "N.*" "O.*" "S.*") and (not backbone)







Working on an illustration

Selections Tab

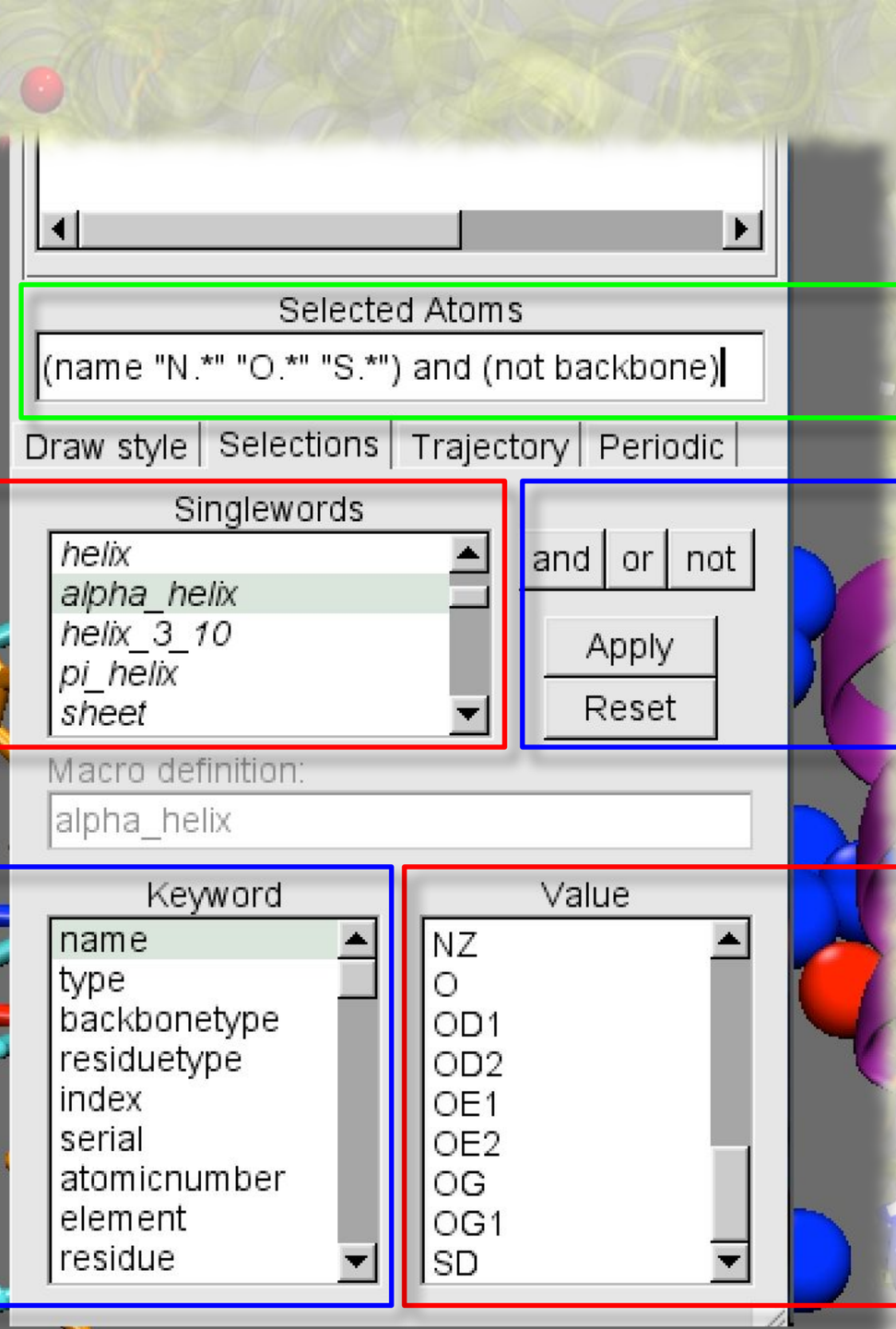
Current selection

Single word **predefined** selections

Input buttons

List of data fields, **keywords**

List of **values** for a selected **keyword**



VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

1: speptide cartoon

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all
VDW	Name	(name "N.*"

Selected Atoms

(name "N.*" "O.*" "S.*") and (not backbone)

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Glass1

Drawing Method: VDW

Default

Sphere Scale: 0.4

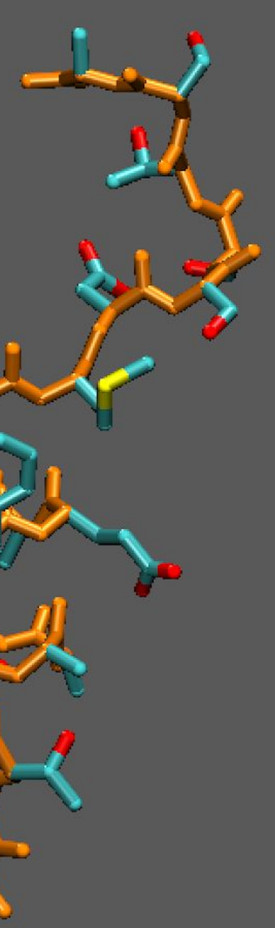
Sphere Resolution: 12

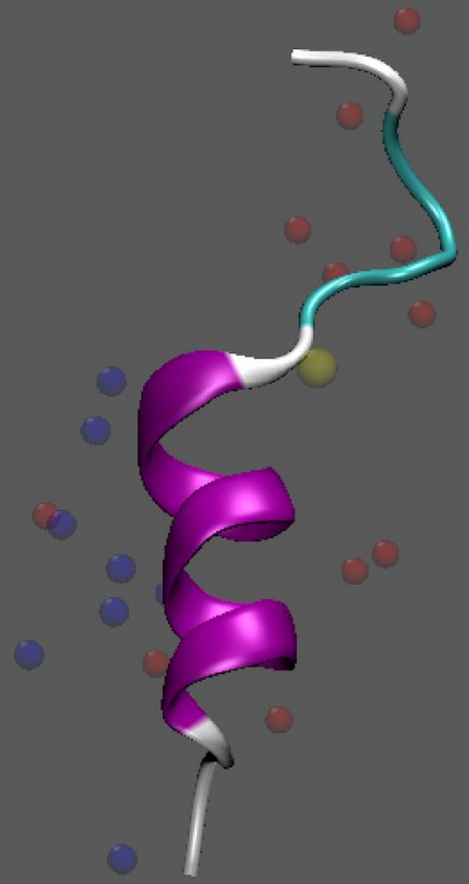
Apply Changes Automatically Apply

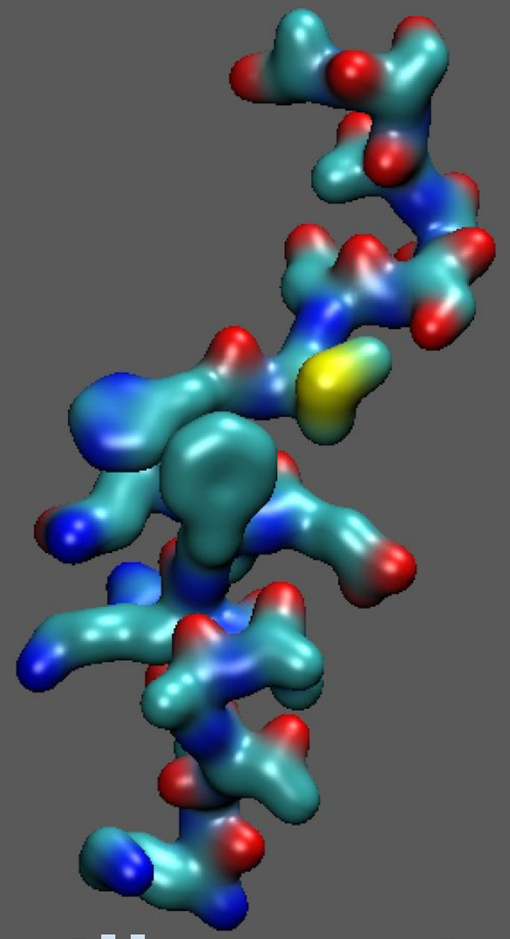
VMD 1.9.3 OpenGL Display

y z x

- Make the new representation less obtrusive.
- Material: **Glass1**;
- Sphere scale: **0.4**;







Working on an illustration

VMD File Edit — 100% Sun Mar 3 15:28:12

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0 zoom Loop step 1 speed

Graphical Representations

Selected Molecule

1: speptide cartoon

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all
VDW	Name	(name "N.*"
Licorice	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Drawing Method: Licorice

Material: Glass1

Default

Sphere Resolution 12

Bond Radius 0.1

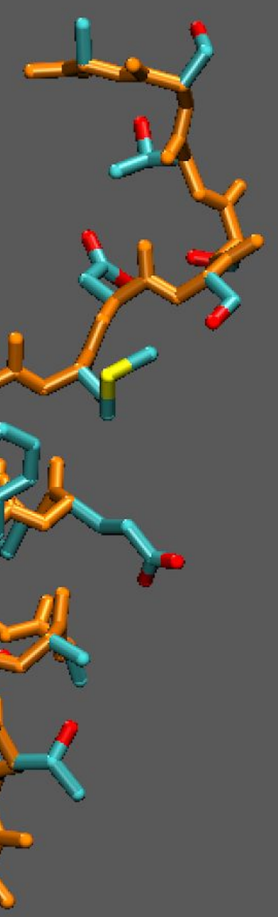
Bond Resolution 12

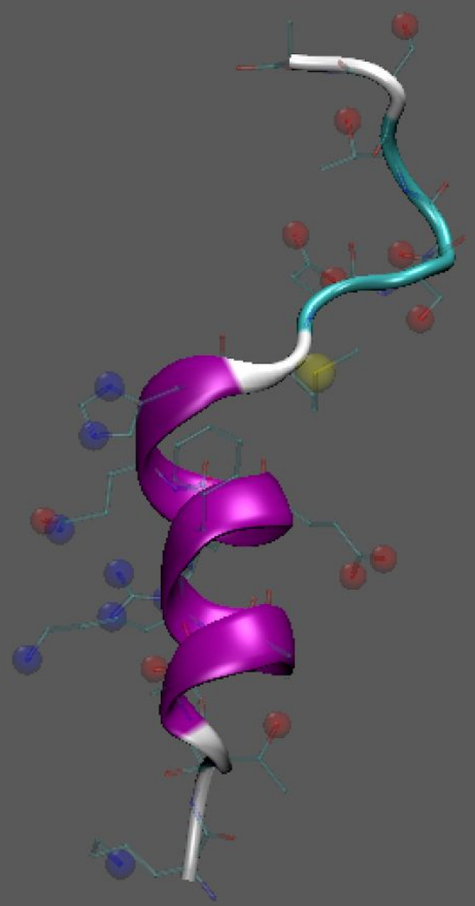
Apply Changes Automatically Apply

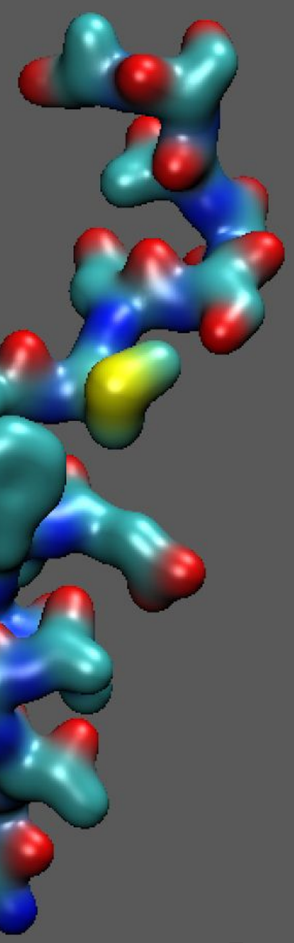
VMD 1.9.3 OpenGL Display

y x z

- Let us give a hint of the **connectivity** for the new atoms.
- **New** representation: **All**, **Licorice**, **Name**.
- Material: **Glass1**;
- Bond Radius: 0.3 -> **0.1**;







Working on an illustration

VMD File Edit

100% Sun Mar 3 15:29:30

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Graphical Representations

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style	Color	Selection
QuickSurf	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Glossy

Drawing Method: QuickSurf

Default

Resolution 0.50

Radius Scale 0.5

Density Isovalue 0.5

Grid Spacing 0.2

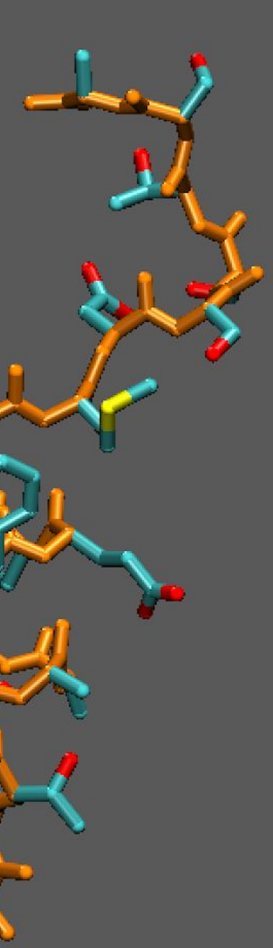
Surface Quality Max

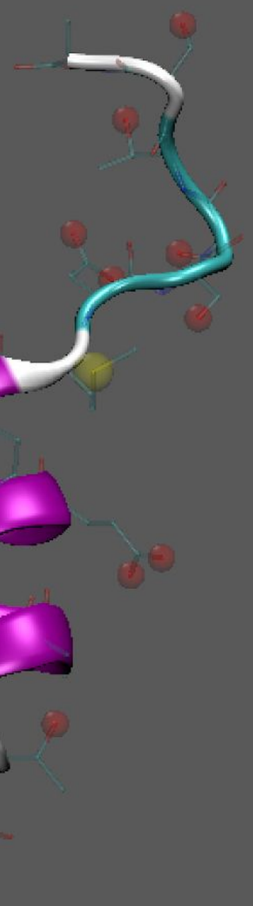
Apply Changes Automatically Apply

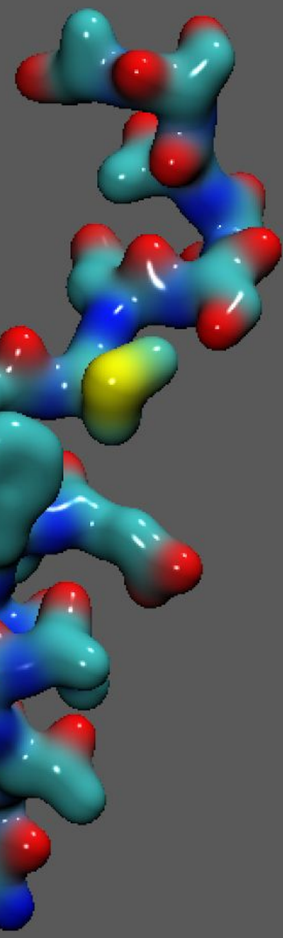
VMD 1.9.3 OpenGL Display

y x z

- Make the “**volume**” molecule better looking;
- Material: **Glossy**.







Working on an illustration

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID T A D F Molecule

0 A D F speptide structure
1 A D F speptide cartoon
2 T A D F speptide volume

Rotate Mode R
Translate Mode T
Scale Mode S
Center
Query 0
Label
Move
Force
Add/Remove Bonds
Pick P

Atoms 1
Bonds 2
Angles 3
Dihedrals 4

zoom Loop step

Selected Molecule
2: speptide volume

Create Rep Delete Rep

Style Color Selection
QuickSurf Name all

Selected Atoms
all

Draw style | Selections | Trajectory | Periodic

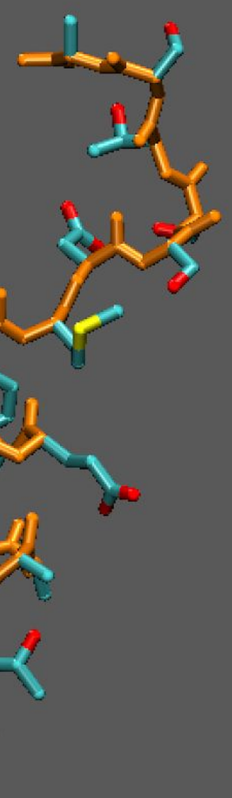
Coloring Method: Name
Material: Glossy
Drawing Method: QuickSurf
Default

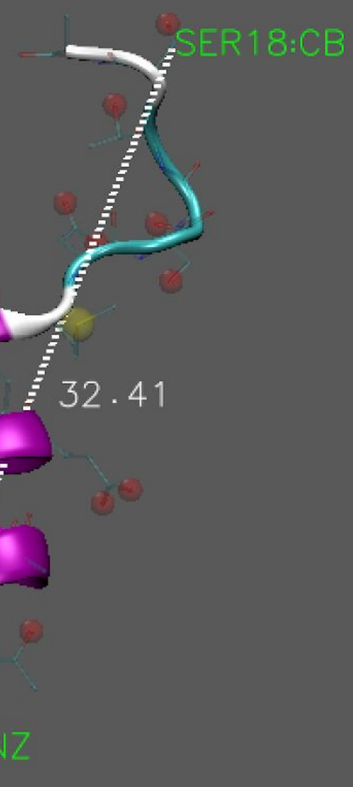
Resolution 0.50
Radius Scale 0.5
Density Isovalue 0.5
Grid Spacing 0.2
Surface Quality Max

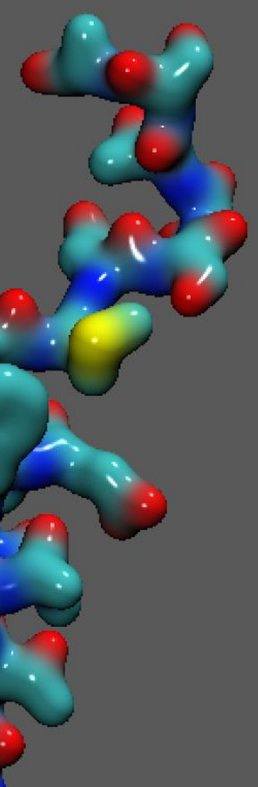
Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

- Let us get a **sense of size** by adding a measure.
- Mouse mode: **Label** / **Bonds**.
- Click **two atoms** at the opposite ends of the "**cartoon**" molecule.







Working on an illustration

VMD File Edit

100% Sun Mar 3 15:35:17

VMD Main

File Molecule Graphics Display Mouse Extensions Help

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0		A	D	F	speptide structure	146	1	0
1		A	D	F	speptide cartoon	146	1	0
2	T	A	D	F	speptide volume	146	1	0

0 zoom Loop step 1 speed

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style Color Selection

QuickSurf Name all

all

Draw style Sele

Coloring Meth

Name

Drawing Meth

QuickSurf

Resolution 0.5

Ra

Density Isovalue 0.5

Grid Spacing 0.2

Surface Quality Max

Apply Changes Automatically Apply

Labels

Atoms Show Hide Delete

SER18:CB
LYS1:NZ

Picked Atom Graph Properties Global Properties

Molecule: 1: speptide cartoon

XYZ: 21.589 0.757 25.825

ResName: LYS Chain: X

ResID: 1 SegName: 1SRN

Name: NZ Index: 8

Type: NZ Value: 0.000

VMD 1.9.3 OpenGL Display

y x z

Labels control window

- Bring up **Labels** floating dialog from **Graphics** menu.
- Remove the **atomic labels**;
- Leave the **bond label** in place.

SER18:CB

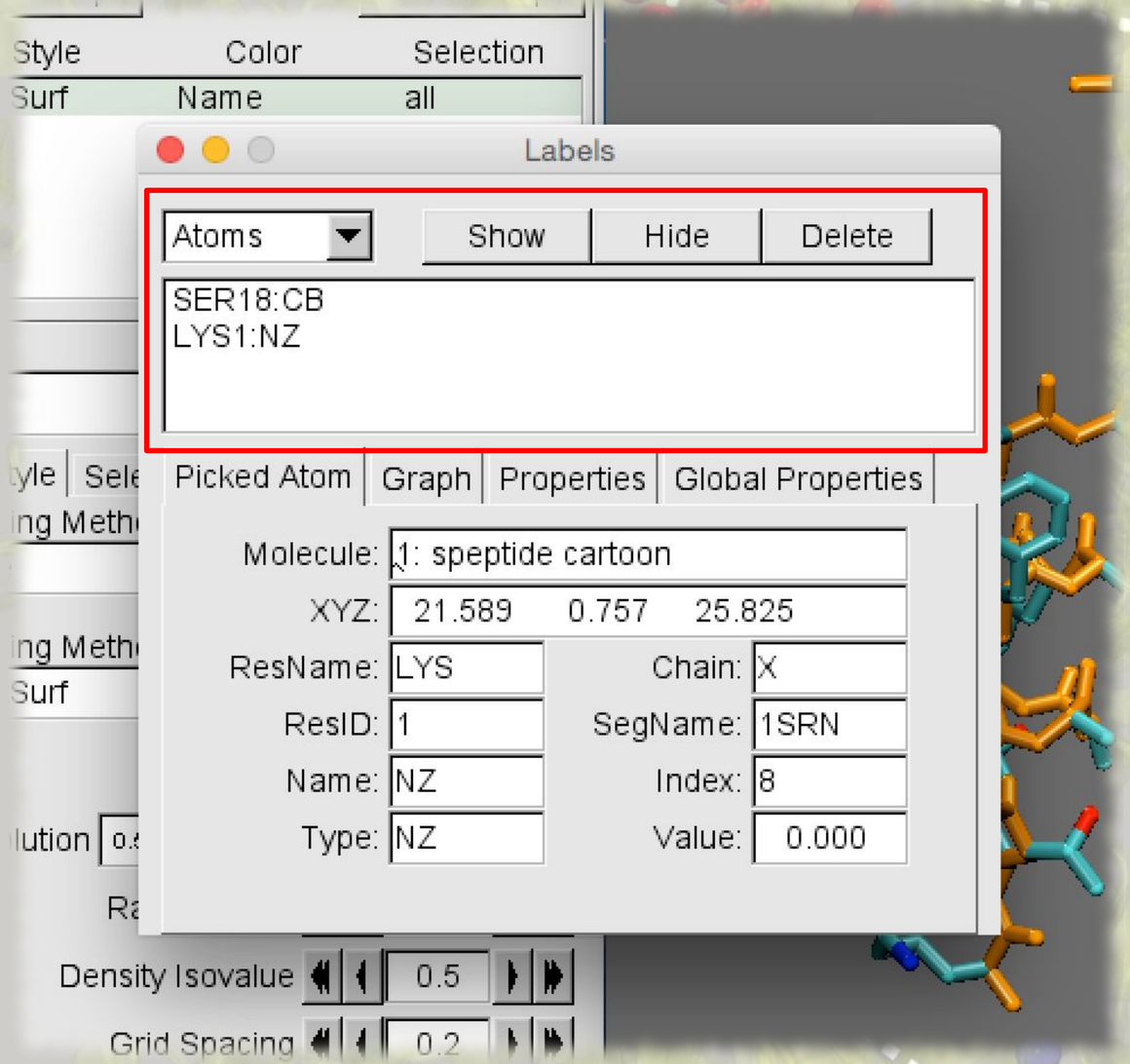
32.41

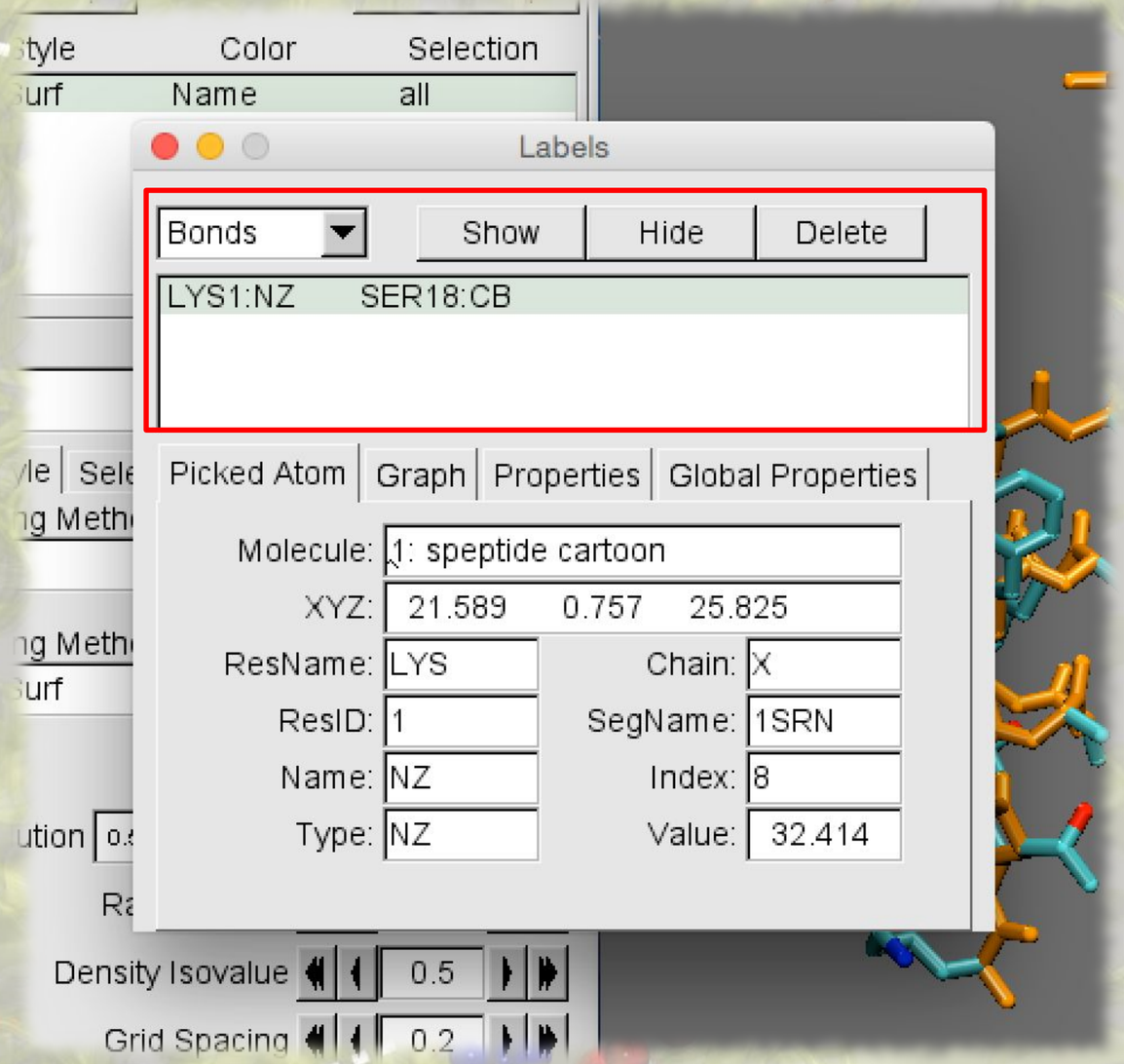
LYS1:NZ

Working on an illustration

Labels control

Floating dialog.
Stays until closed.





- Delete atomic labels;
- Keep the bond label.

VMD File Edit

100% Sun Mar 3 15:39:10

VMD Main

File Molecule Graphics Display Mouse

ID	T	A	D	F	Molecule	Atoms
0		A	D	F	speptide structure	146
1		A	D	F	speptide cartoon	146
2	T	A	D	F	speptide volume	146

0

zoom Loop step 1 speed

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style	Color	Selection
QuickSurf	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Name

Material: Glossy

Drawing Method: QuickSurf

Default

Resolution 0.50

Radius Scale 0.5

Density Isovalue 0.5

Grid Spacing 0.2

Surface Quality Max

Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

y

z x

32.41

Done.

VMD File Edit

100% Sun Mar 3 16:59:48

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
re	146	1	0
h	146	1	0
	146	1	0

1 speed

0: peptide structure

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all
Licorice	ColorID 3	backbone

Selected Atoms

backbone

Draw style | Selections | Trajectory | Periodic

Coloring Method: ColorID 3 Material: Opaque

Drawing Method: Licorice Default

Sphere Resolution 12

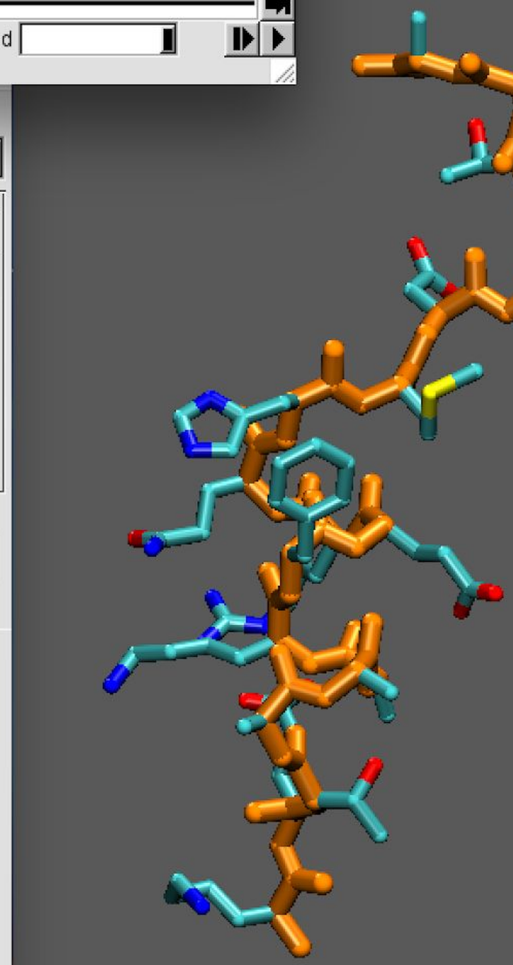
Bond Radius 0.4

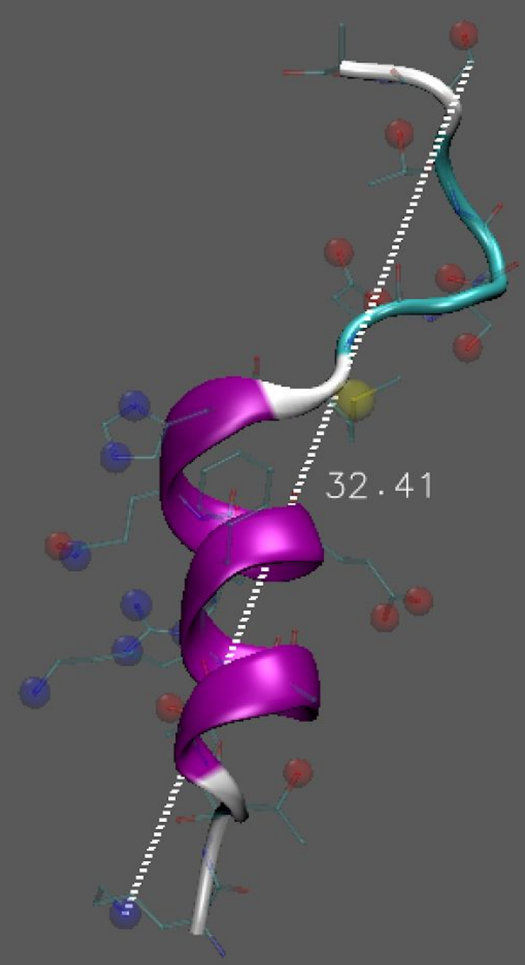
Bond Resolution 12

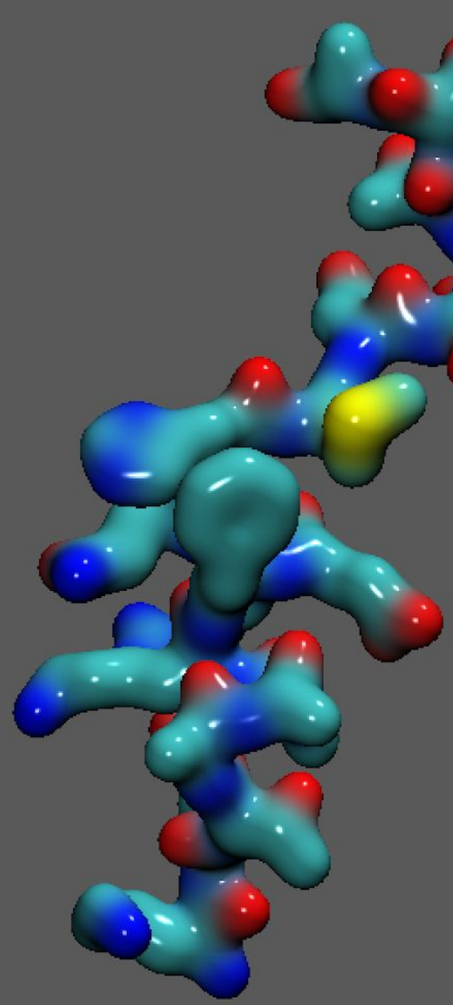
Apply Changes Automatically Apply

VMD 1.9.3 OpenGL Display

- Final image can be generated by the **Render** option from the **File** menu.

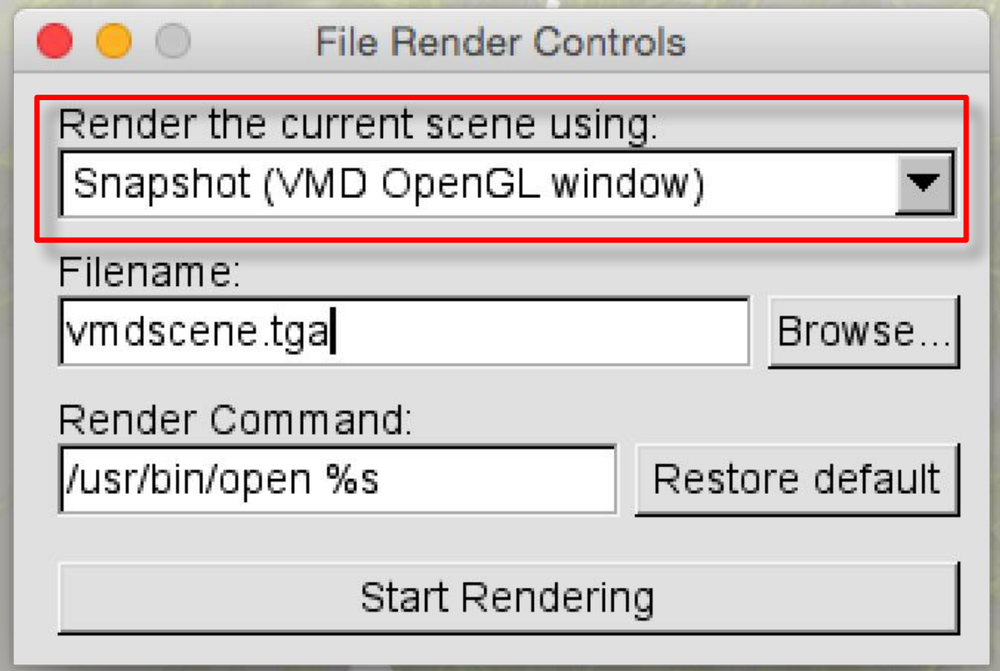


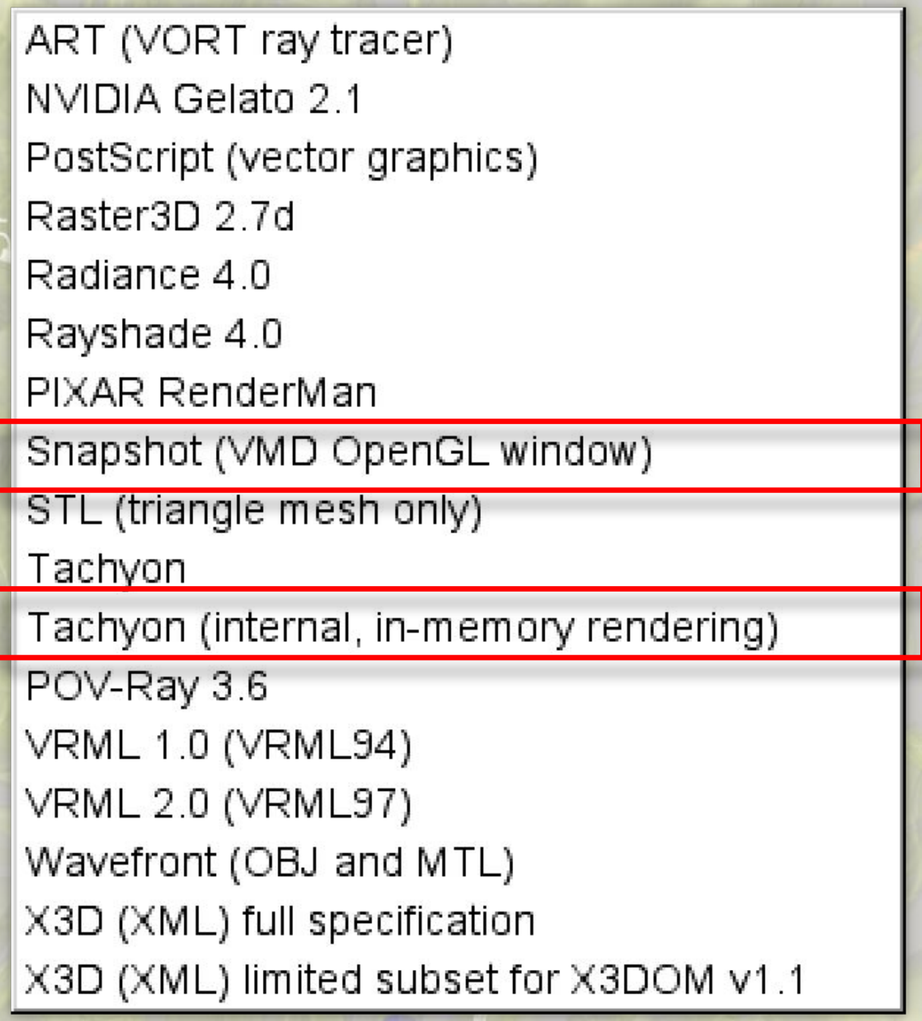




Render it.

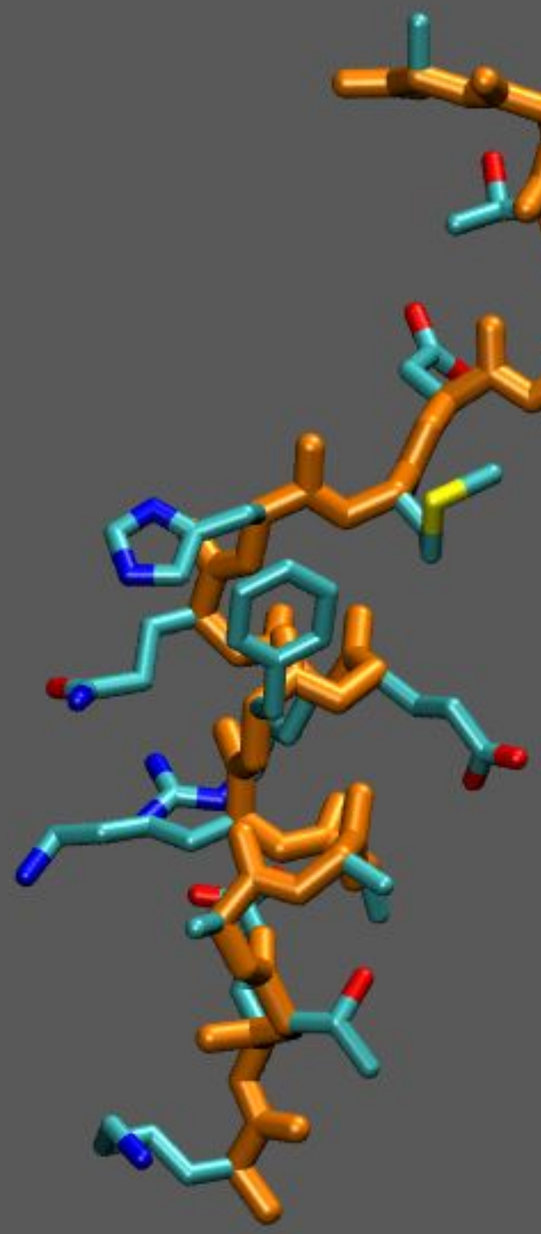
Render dialog

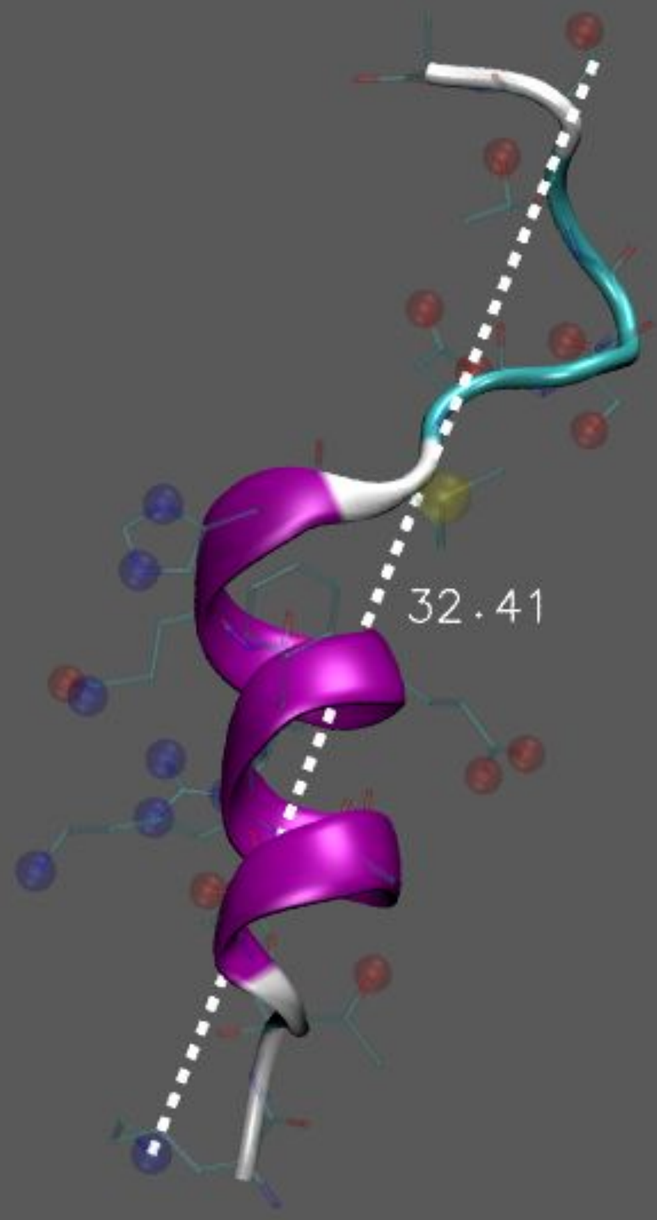


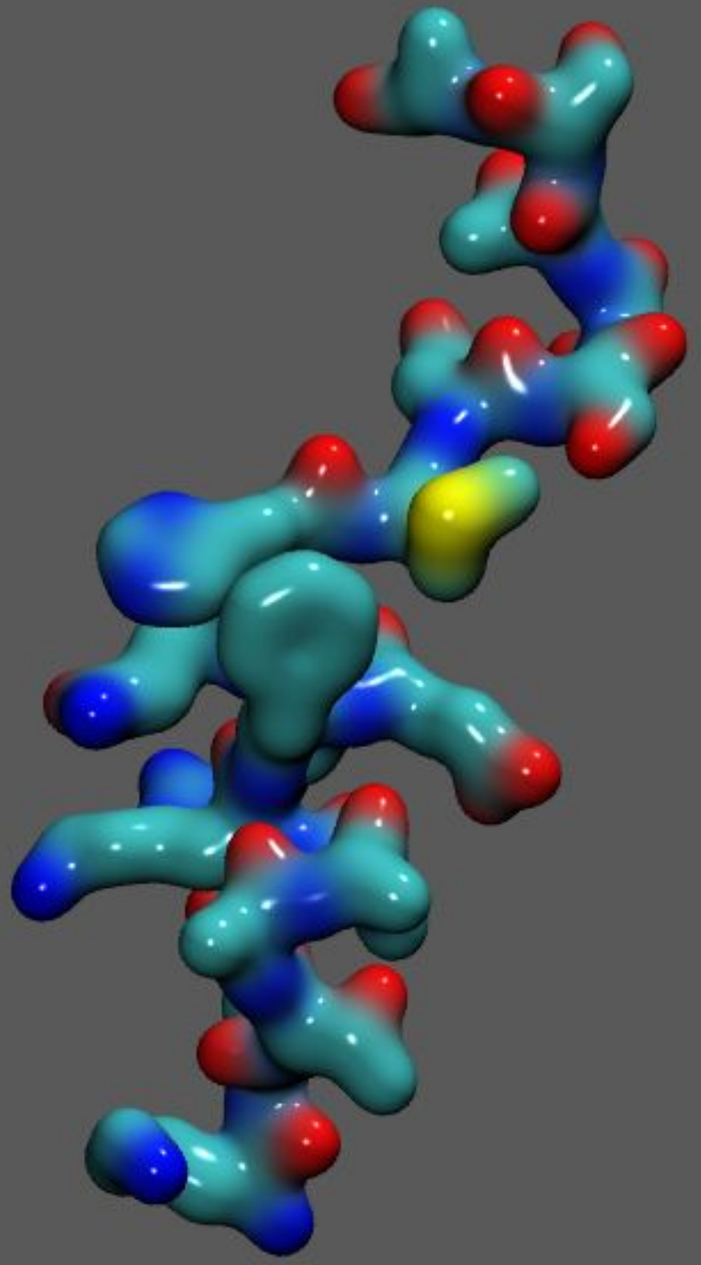


- Internal and External renderers.
- External renderers require additional software.
- Internal (included) options are normally enough.

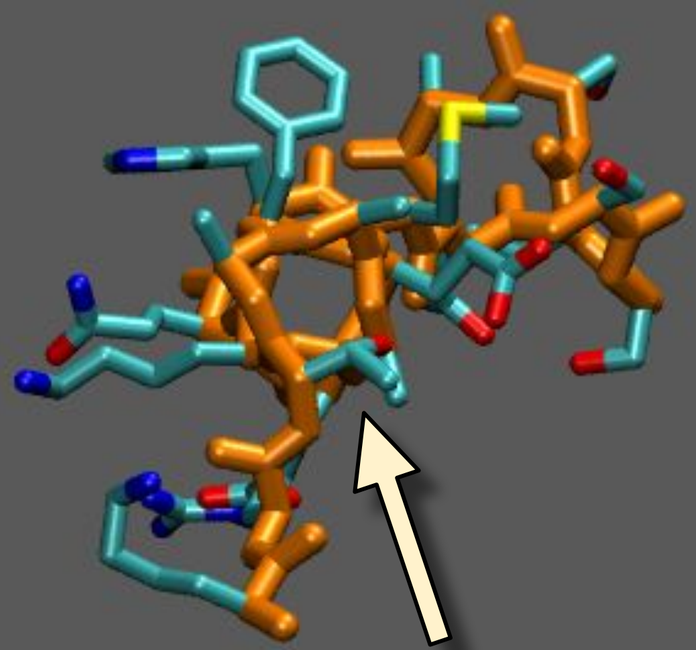
Tachyon ray traced image

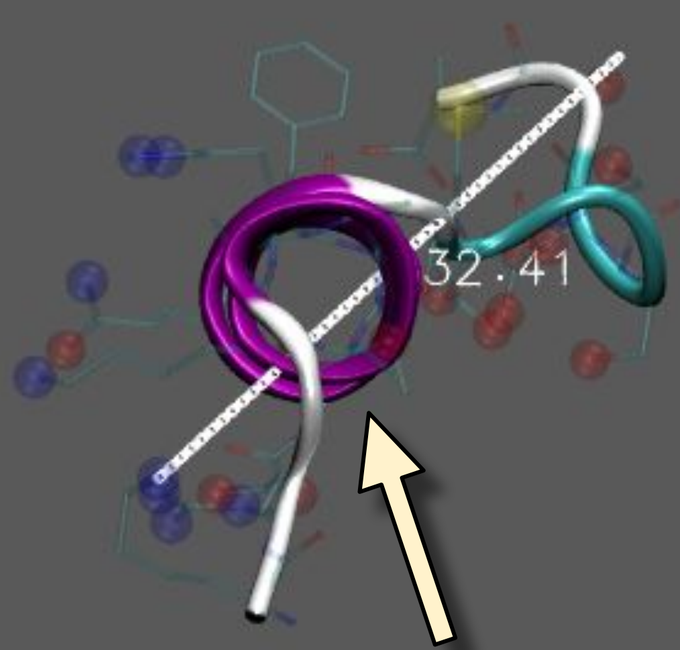


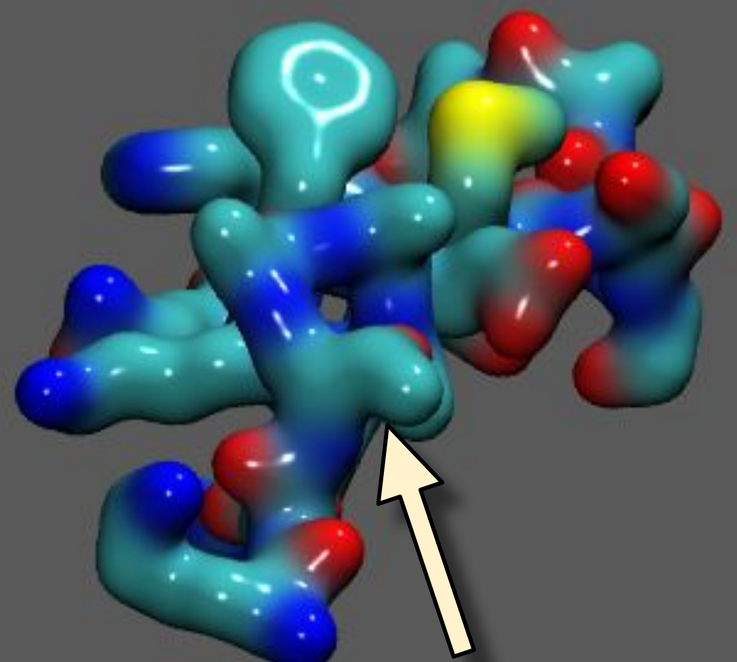




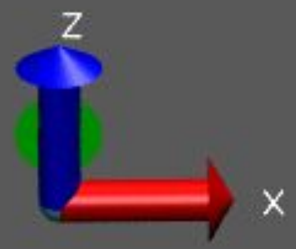
Helix channel view







Helix Inner Channel



VMD resources

- VMD Home: http://www.ks.uiuc.edu/Research/vmd/
- FAQ: http://www.ks.uiuc.edu/Research/vmd/allversions/vmd_faq.html
- VMD Documentation: https://www.ks.uiuc.edu/Research/vmd/current/docs.html
- VMD on Compute Canada: https://docs.computecanada.ca/wiki/VMD

Data sources:

- PDB Data Bank: https://www.wwpdb.org
- Nucleic Acids Data Bank: http://ndbserver.rutgers.edu

Thank you!