

# Molecular visualization with VMD

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# 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>

VMD is Copyright ©  
1995-2016 **Theoretical  
and Computational  
Biophysics Group** and at  
the **University of Illinois**.

## Registration/Login

You will need a username and password to download software.

**If this is your first download, please choose a username and password to register.**

Current NAMD or VMD users, please enter your existing username and password.

Username:

Password:

Continue with registration or download

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

## 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>

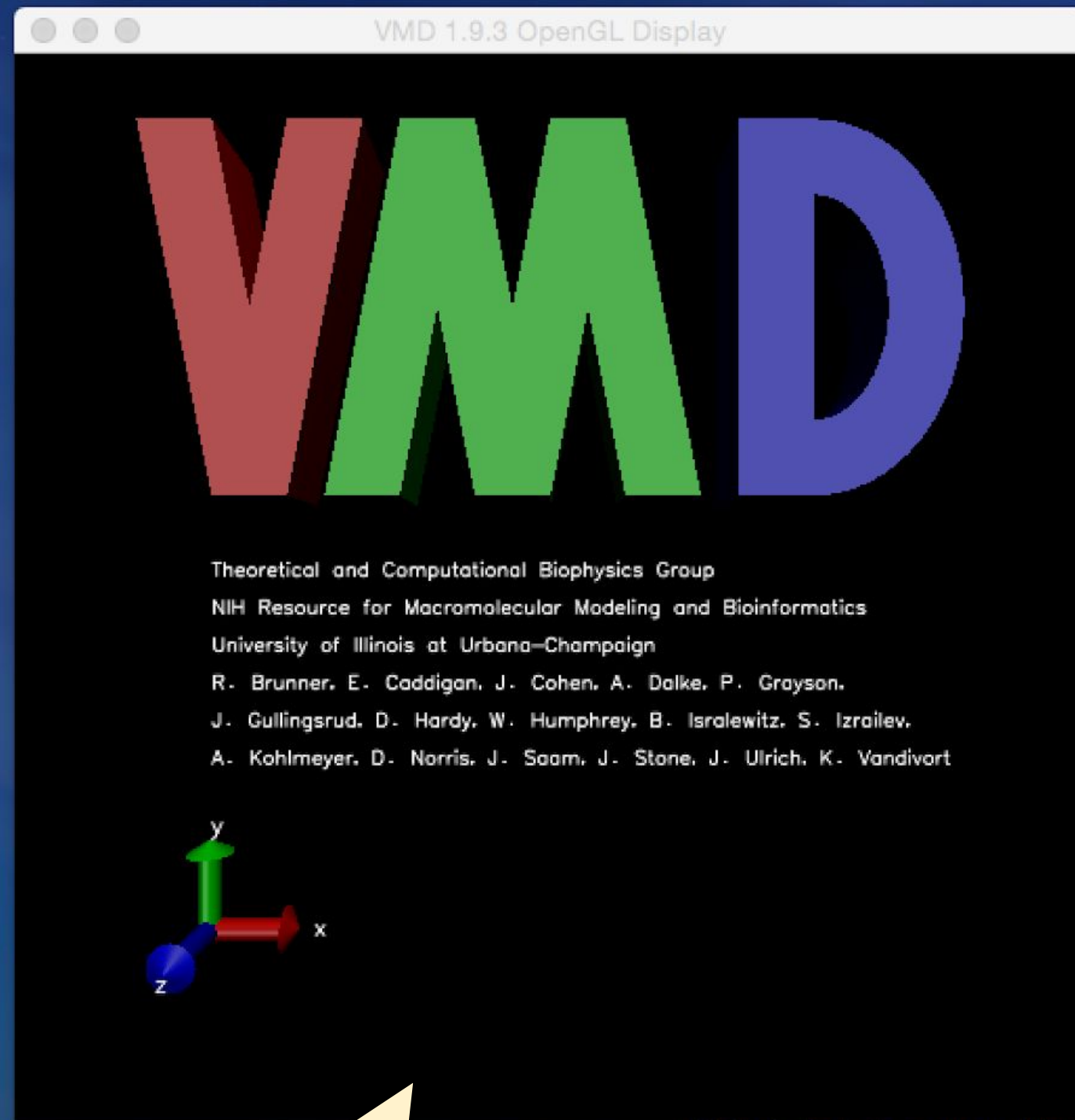


# Overview of VMD related topics

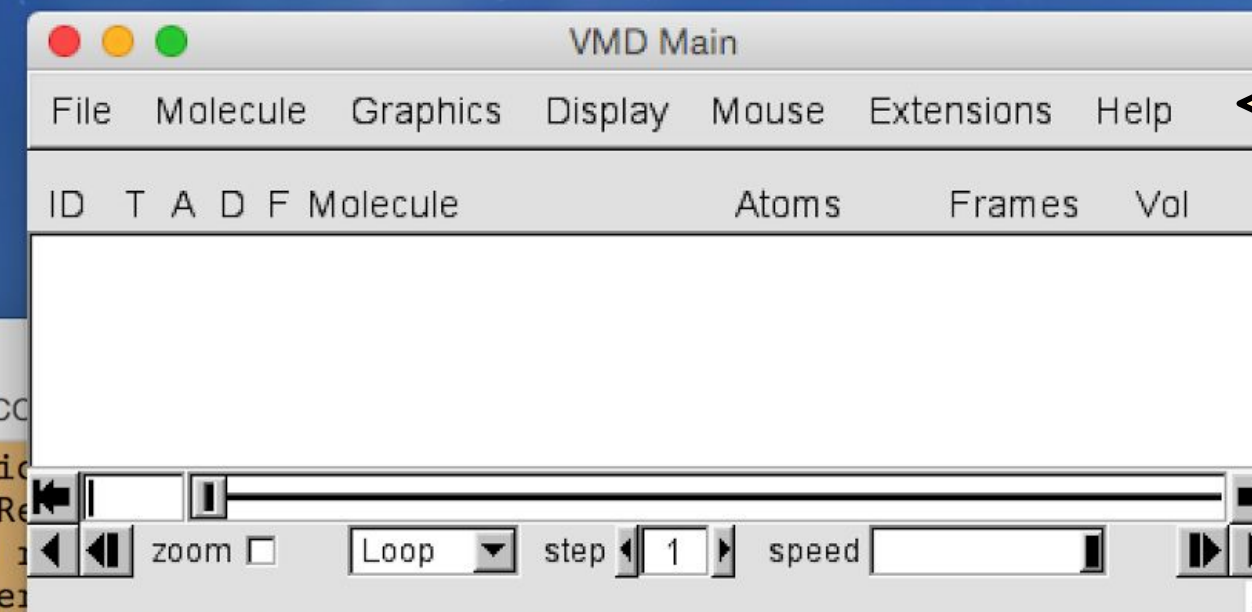
- **Basic techniques**
  - **Molecules and representations.**
  - **3D navigation.**
  - **Drawing methods.**
  - **Materials and coloring.**
  - **Atom selection techniques.**
- Working with trajectories.
- Creating animations and movies.
- Scripting and automation.
- **Rendering high quality images.**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



# Starting VMD



OpenGL graphics window



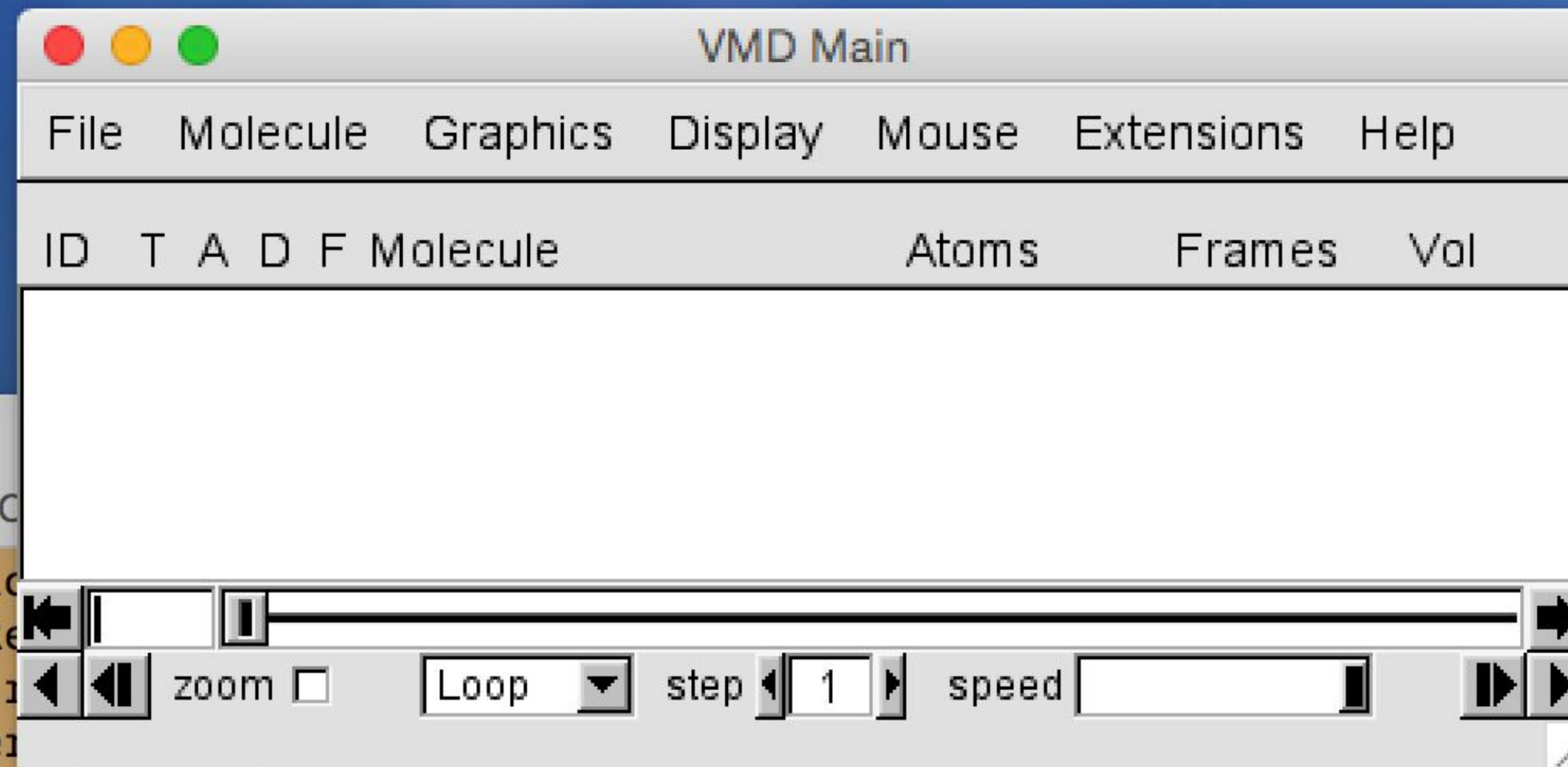
Main control window

```
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



## 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

## Display

- 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...

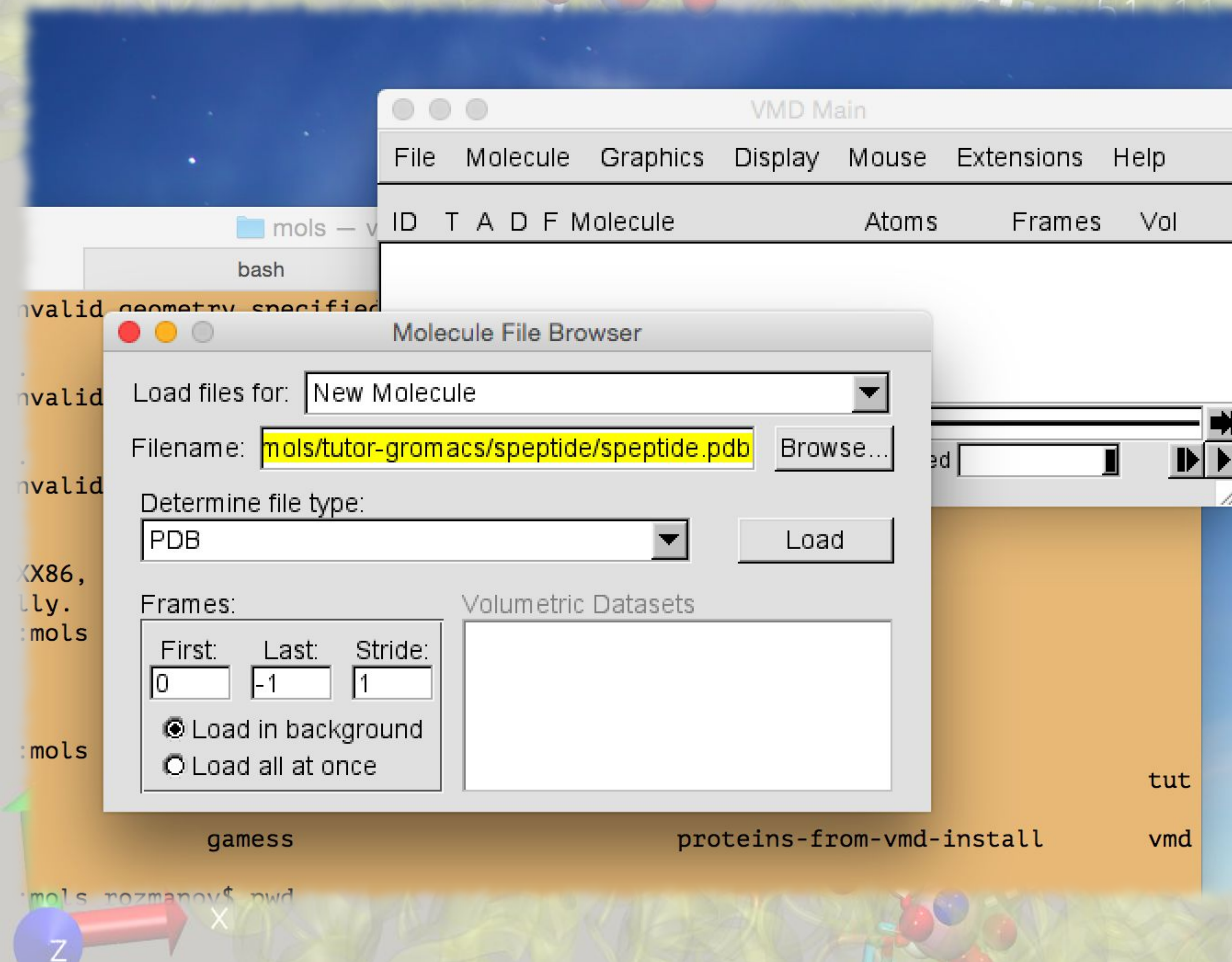
## Extensions

- 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.**

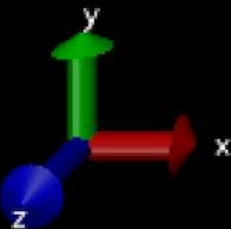
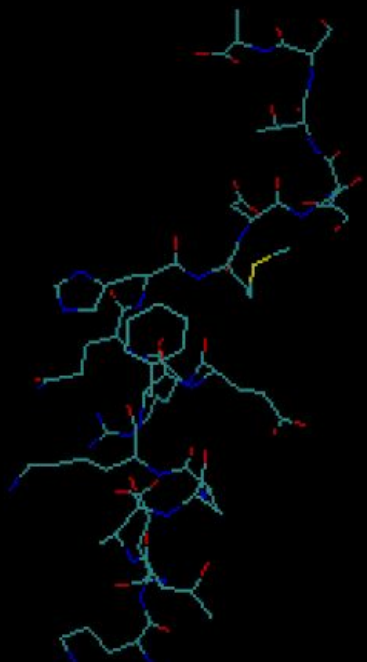




# Loading a molecule

## 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

Loaded molecule

```
vmd_MACOSXX86
e this refer
W., Dalke,
Dynamics', 3. notes: Graphics 1990, 1991, 95-98.

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 Improvers: 0 Cross-terms: 0
Info) Bondtypes: 0 Angletypes: 0 Dihedraltypes: 0 Improptypes: 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

ID - molecule number.

T - “Top” stat.

A - Active.

D - Drawn.

F - Fixed.

# of Atoms.

# of Frames.

Volumetric data.

VMD Main

File Molecule Graphics Display Mouse Extensions Help

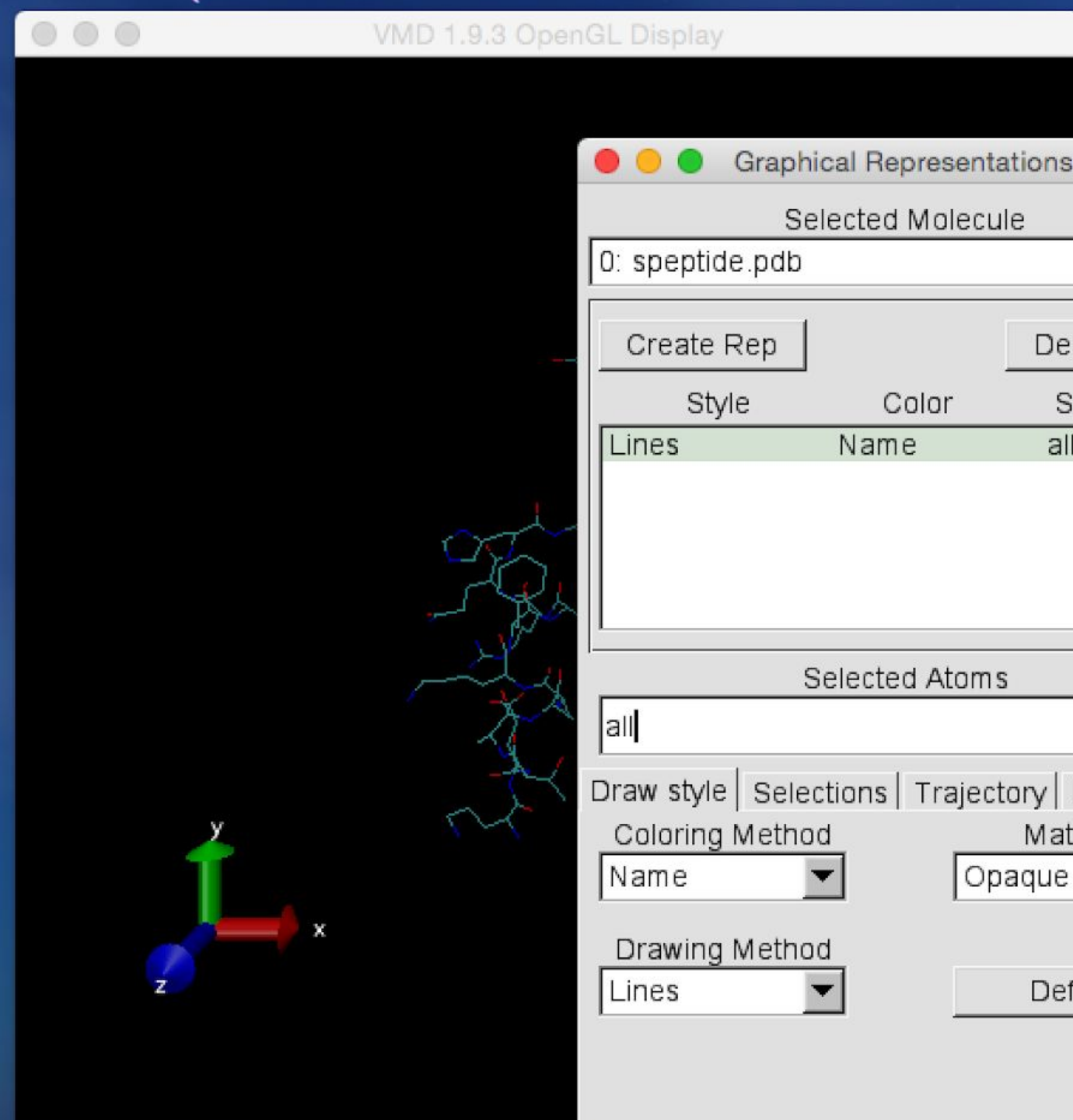
ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

Navigation controls: back, forward, zoom, Loop, step, speed, play, pause, stop.

Trajectory animation controls



# Working with a single molecule



Graphical Representations

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 Main

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

Graphical  
Representations  
window



xx86  
fe  
,  
, 3. notes: Graphics 1978, 1971, 99-98.  
-----  
le, 8 CPUs detected.  
A GeForce GT 750M OpenGL Engine  
E CVA MTX NPOT PP PS GLSL(OVF)  
mode is available.  
x16384), 3-D (2048x2048x2048), Multitexture (8)  
lugins in directory:  
3.app/Contents/vmd/plugins/MACOSXX86/molfile  
for structure file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tut  
.pdb  
ordinates from file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tu  
e.pdb  
ture from distance search ...  
.  
s: 0 Improper: 0 Cross-terms: 0  
types: 0 Dihedraltypes: 0 Improptypes: 0  
ein: 1 Nucleic: 0  
te file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tutor-gromacs/s  
peptide/speptide.pdb.  
□



# Representations

Molecule selector.

List of Representations.

Atom selection.

Drawing method,  
Coloring scheme,  
Material controls.

Drawing method  
parameters.

Graphical Representations

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

- Atom selection
- Drawing method
- Coloring method
- Material

A molecule can have  
multiple  
representations.

More options



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 | [Slider] | [Buttons]

zoom ☐ Loop step 1 speed [Slider]

Selected Molecule

0: speptide.pdb

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all

Selected Atoms

all

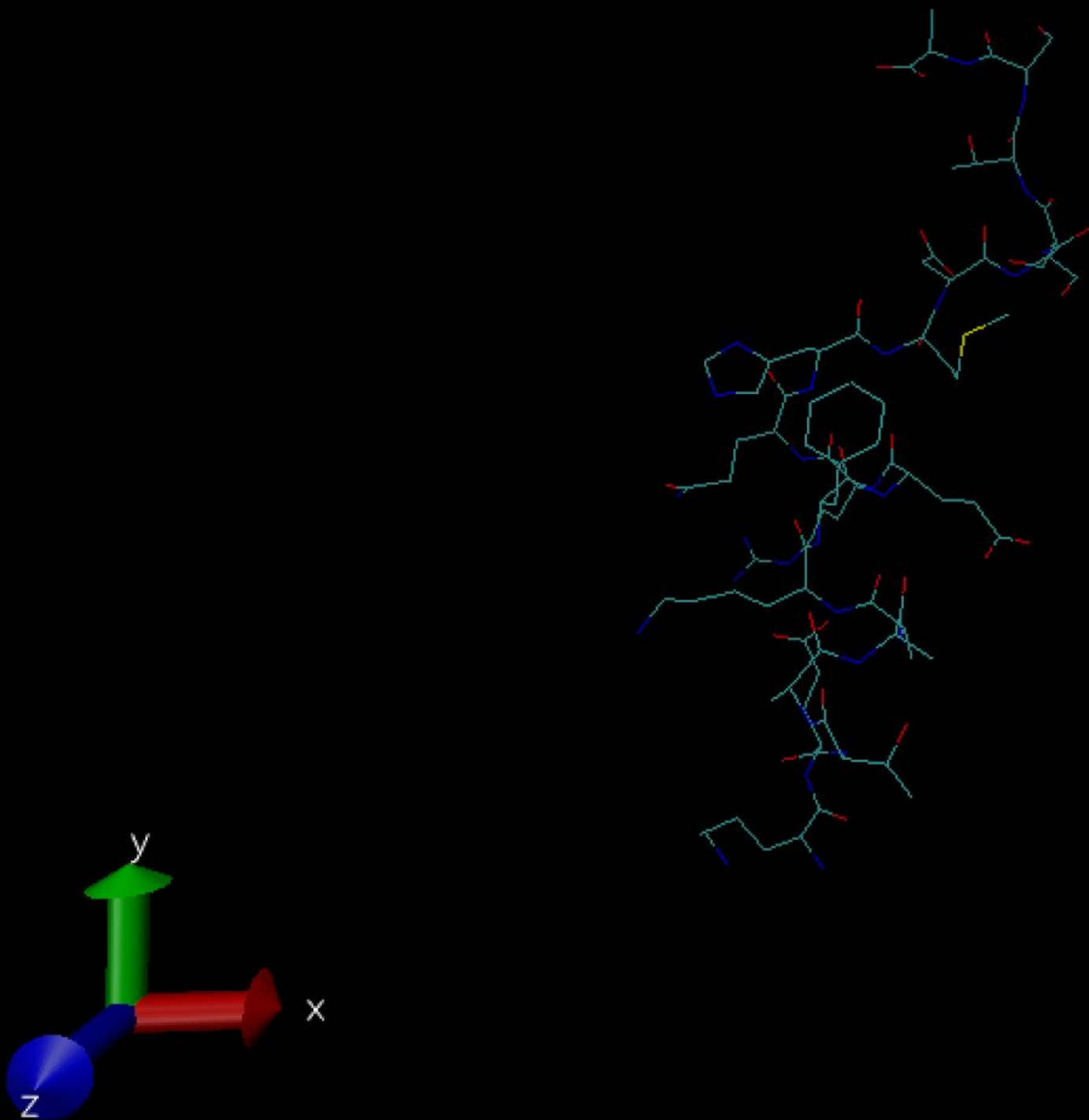
Draw style | Selections | Trajectory | Periodic

Coloring Method: Name Material: Opaque

Drawing Method: Lines Default

Thickness [Slider] 1

◆ Apply Changes Automatically Apply



# Setting up your work space

Distribute the windows to maximize work space.



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 [Slider] [Buttons]

zoom [ ] Loop [ ] step [1] speed [Slider]

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 [Slider]

Apply Changes Automatically [ ] Apply [ ]

# Setting up work space

Color Controls

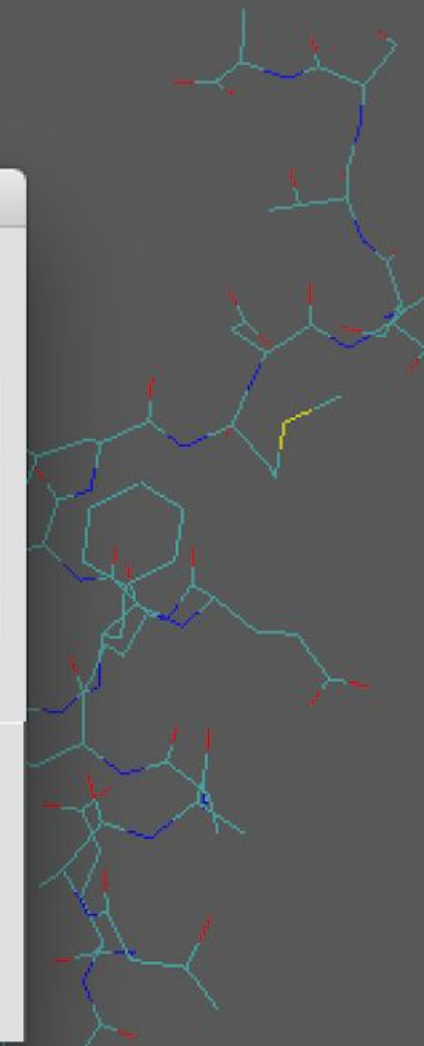
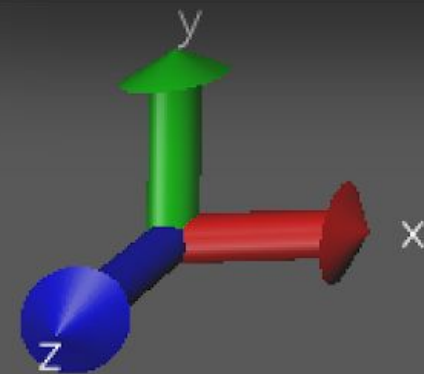
Assign colors to categories:

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	0.35	[Red bar]
1 red	0.35	[Green bar]
2 gray	0.35	[Blue bar]
3 orange		
4 yellow		
5 tan		

Grayscale Default



Colours control window



# Colour control

Floating dialog.  
Stays until closed.

Items and  
Objects

Categories

Colour  
Editor

Colour  
Selector

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	0.35	<div></div>
1 red	0.35	<div></div>
2 gray	0.35	<div></div>
3 orange		
4 yellow		
5 tan		

Grayscale Default



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 | [Progress Bar] | [Buttons]

zoom [ ] Loop [v] step [1] speed [ ] [Buttons]

Graphical Representations

Selected Molecule

0: peptide.pdb

Create Rep   Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

Draw style   Selections   Trajectory   Periodic

Coloring Method: Name [v]   Material: Opaque [v]

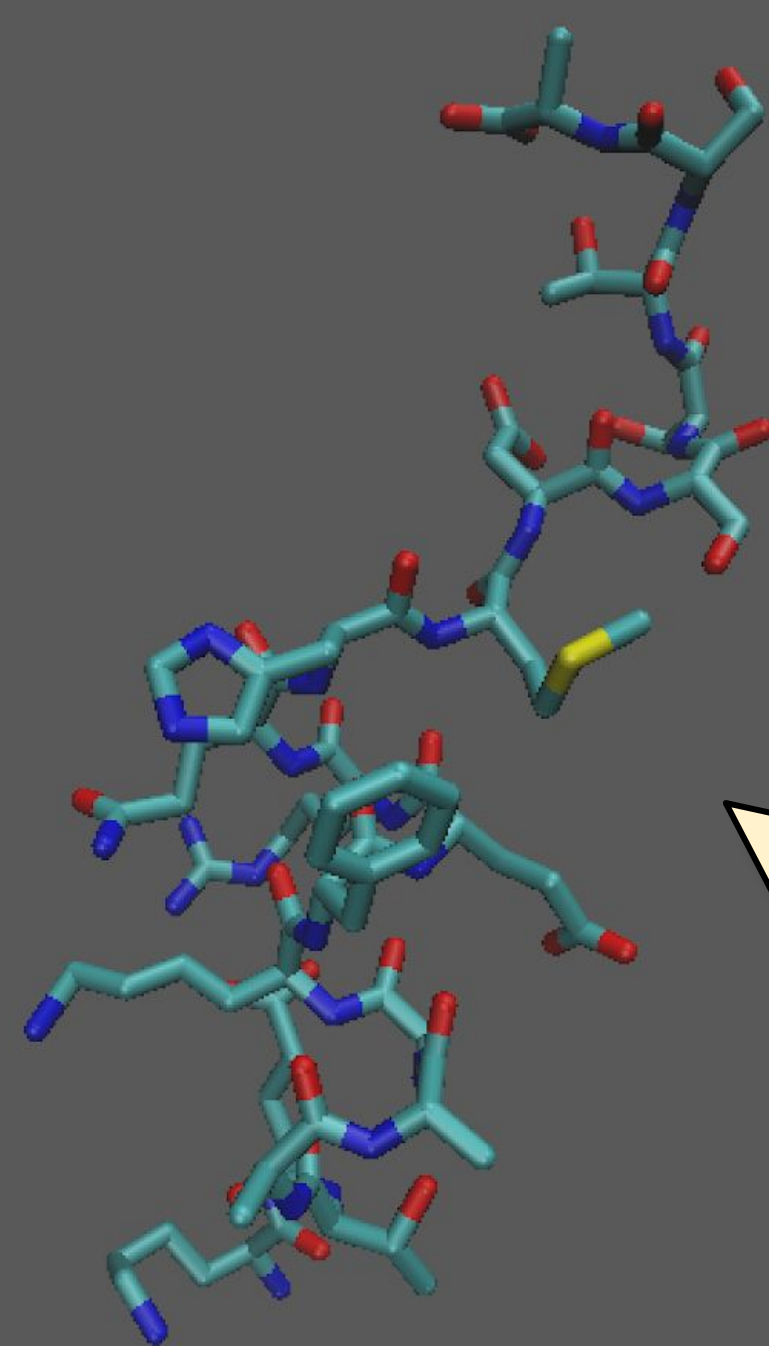
**Drawing Method: Licorice [v]**

Default

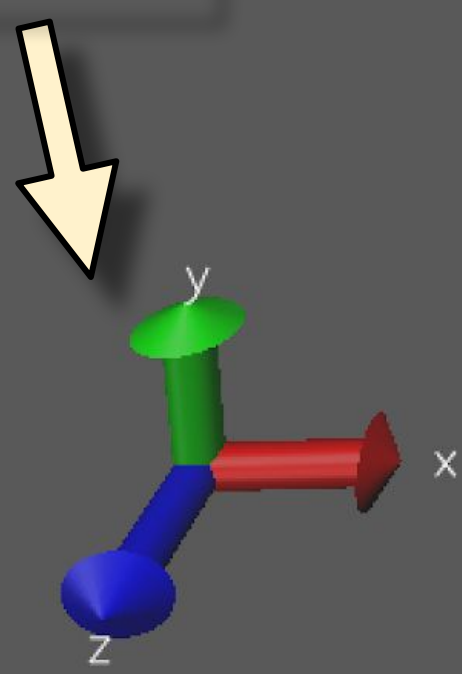
Sphere Resolution [12]   Bond Radius [0.3]   Bond Resolution [12]

Apply Changes Automatically   Apply

# Changing view



3D Axes



Representation of the molecule, "Licorice".







VMD Main

File Molecule Graphics Display Mouse

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

0 [progress bar] zoom [checkbox] Loop [dropdown] step [1] speed [slider]

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

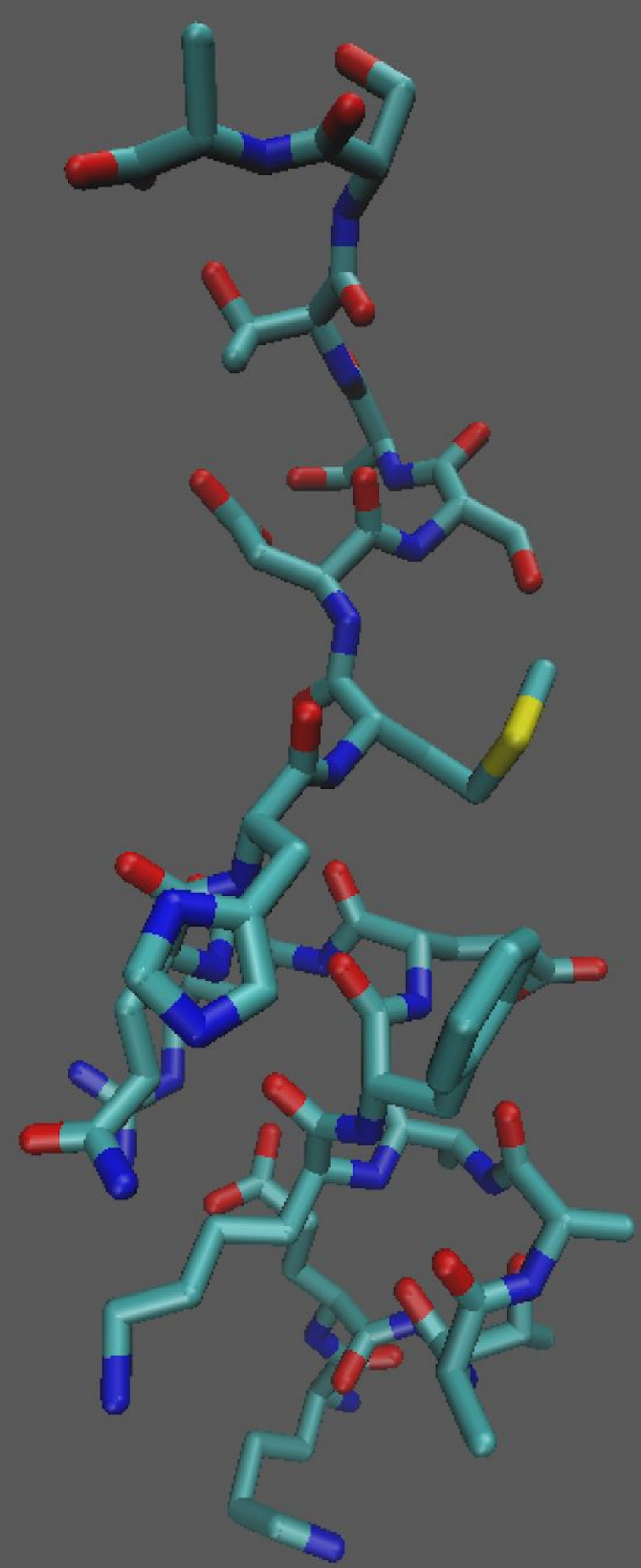
Coloring Method: Name Material: Opaque

Drawing Method: Licorice Default

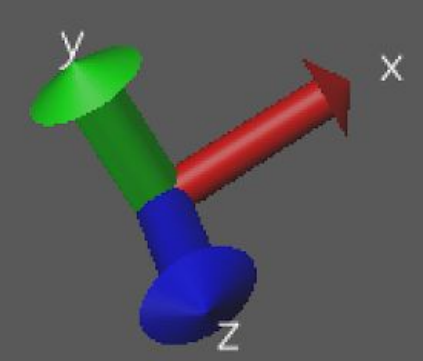
Sphere Resolution: 12 Bond Radius: 0.3 Bond Resolution: 12

Apply Changes Automatically Apply

“R” – rotate  
“T” – translate  
“S” – scale  
“C” – center  
“=” – reset view



<input checked="" type="radio"/> Rotate Mode	R
<input type="radio"/> Translate Mode	T
<input type="radio"/> Scale Mode	S
<input type="radio"/> Center	C
<input type="radio"/> Query	Q
<input type="checkbox"/> Label	
<input type="checkbox"/> Move	
<input type="checkbox"/> Force	
<input type="checkbox"/> Move Light	
<input type="radio"/> Add/Remove Bonds	
<input type="radio"/> Pick	P



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

# Changing view



VMD Main

File   Molecule   Graphics   Display   Mouse

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

0   [Progress Bar]   zoom   [checkbox]   Loop   step   1   speed

● ● ● Graphical Representations

Selected Molecule

0: peptide.pdb

Create Rep   Delete Rep

Style	Color	Selection
VDW	Name	all

Selected Atoms

all

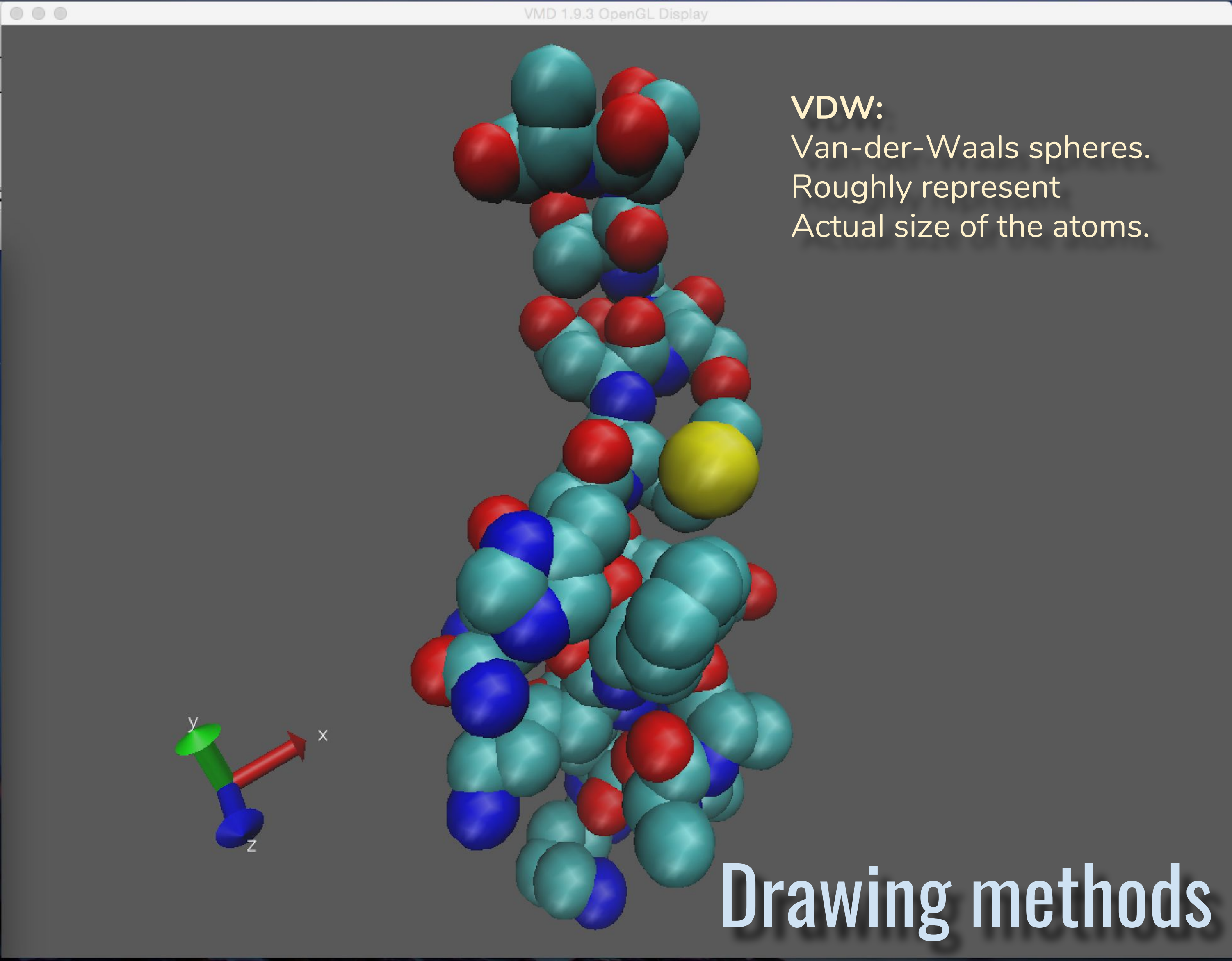
Draw style   Selections   Trajectory   Periodic

Coloring Method: Name   Material: Opaque

Drawing Method: VDW   Default

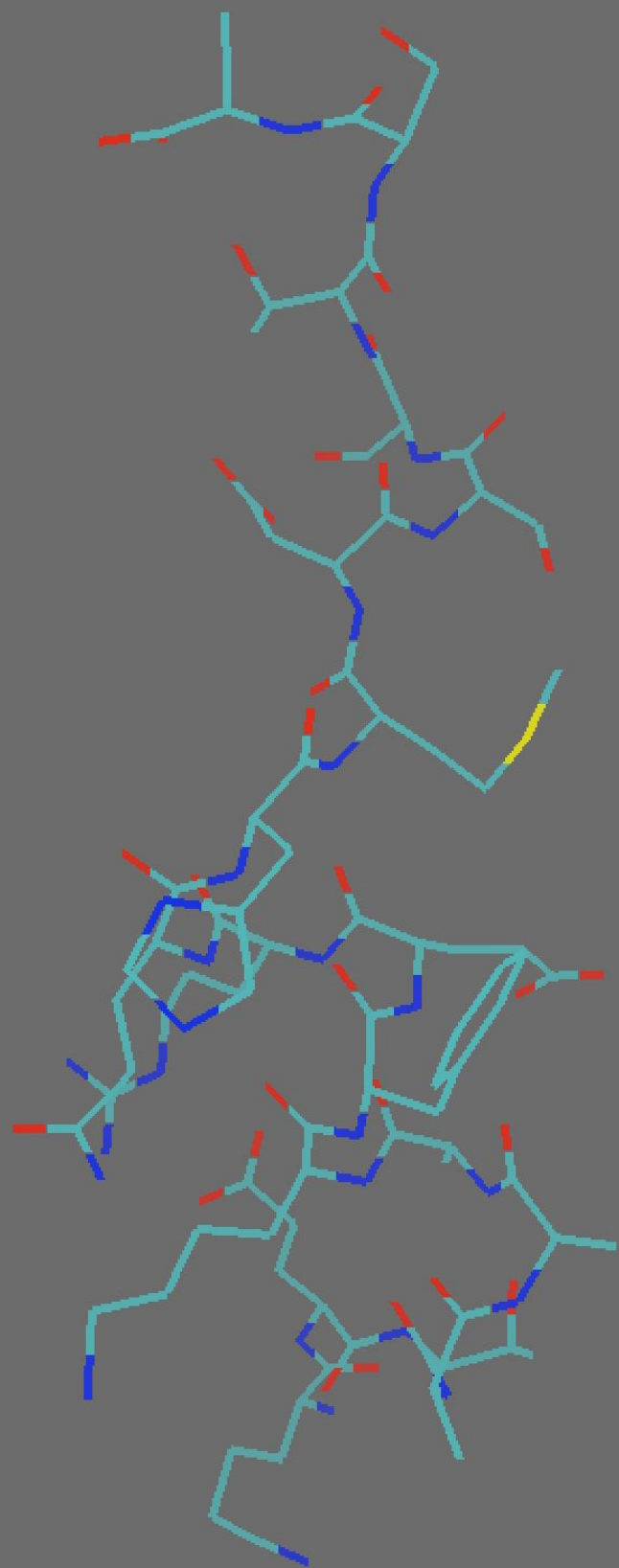
Sphere Scale: 1.0   Sphere Resolution: 12

◆ Apply Changes Automatically   Apply

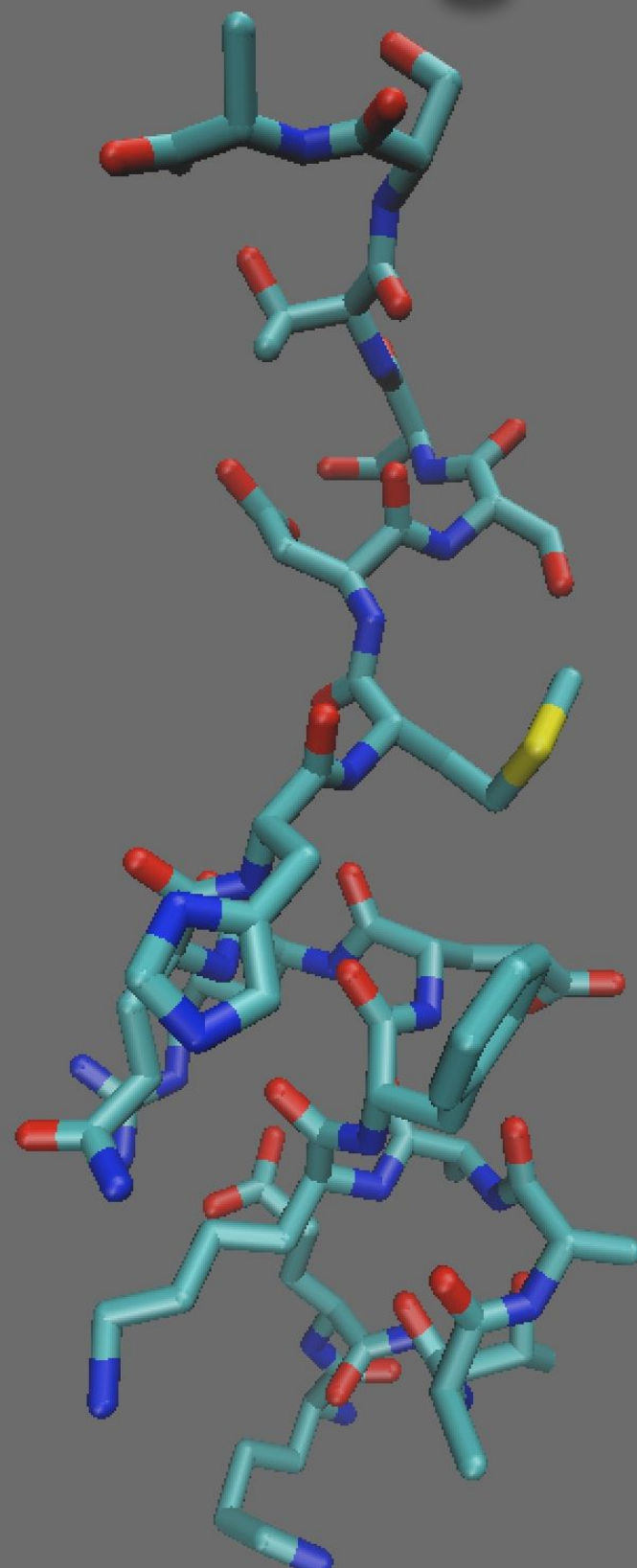




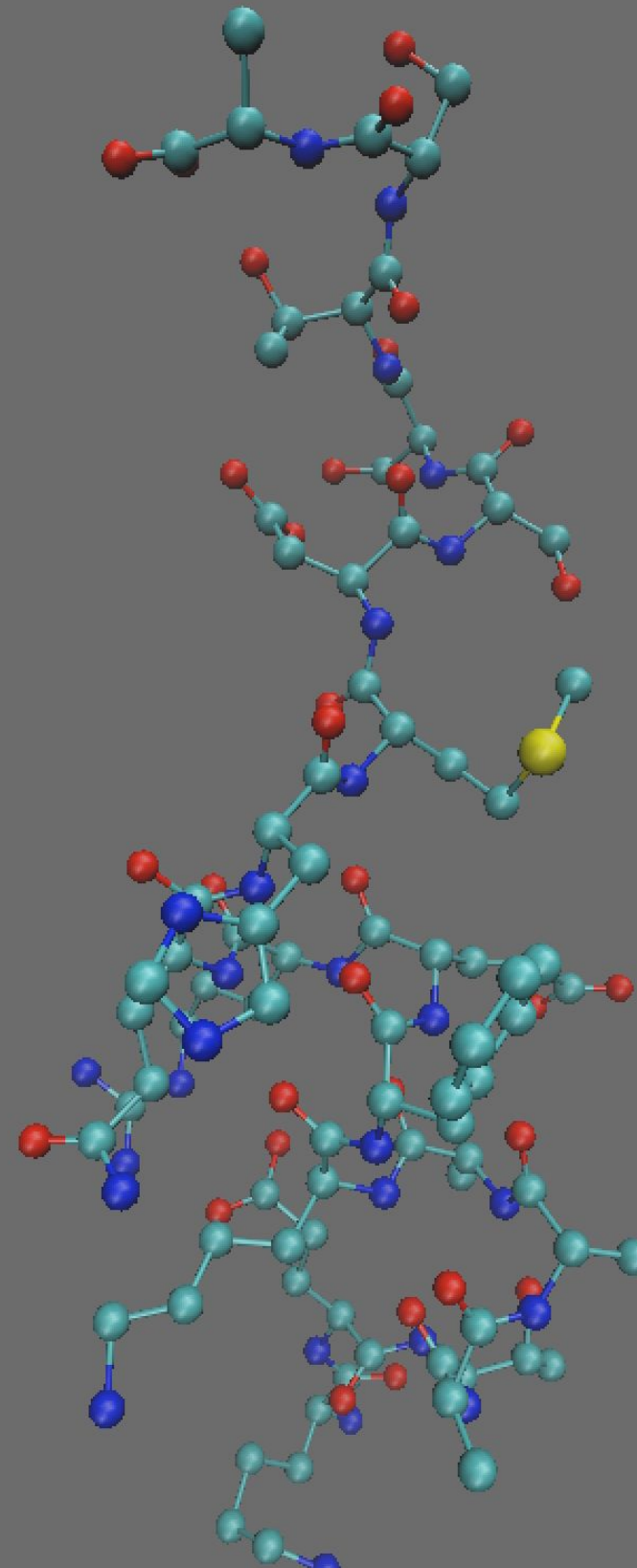
# Atomistic Drawing Methods



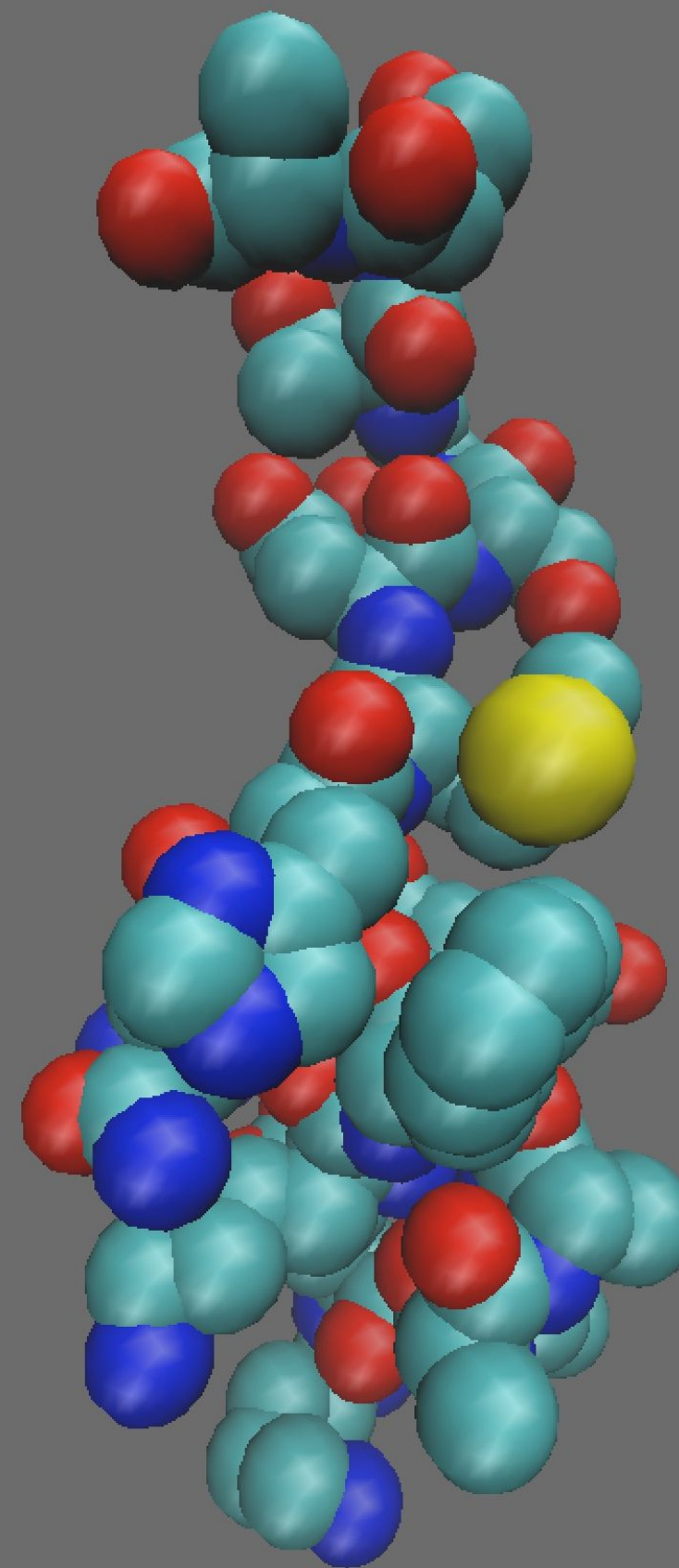
**Lines:**  
Structure, atoms.  
Very lightweight.  
Default.



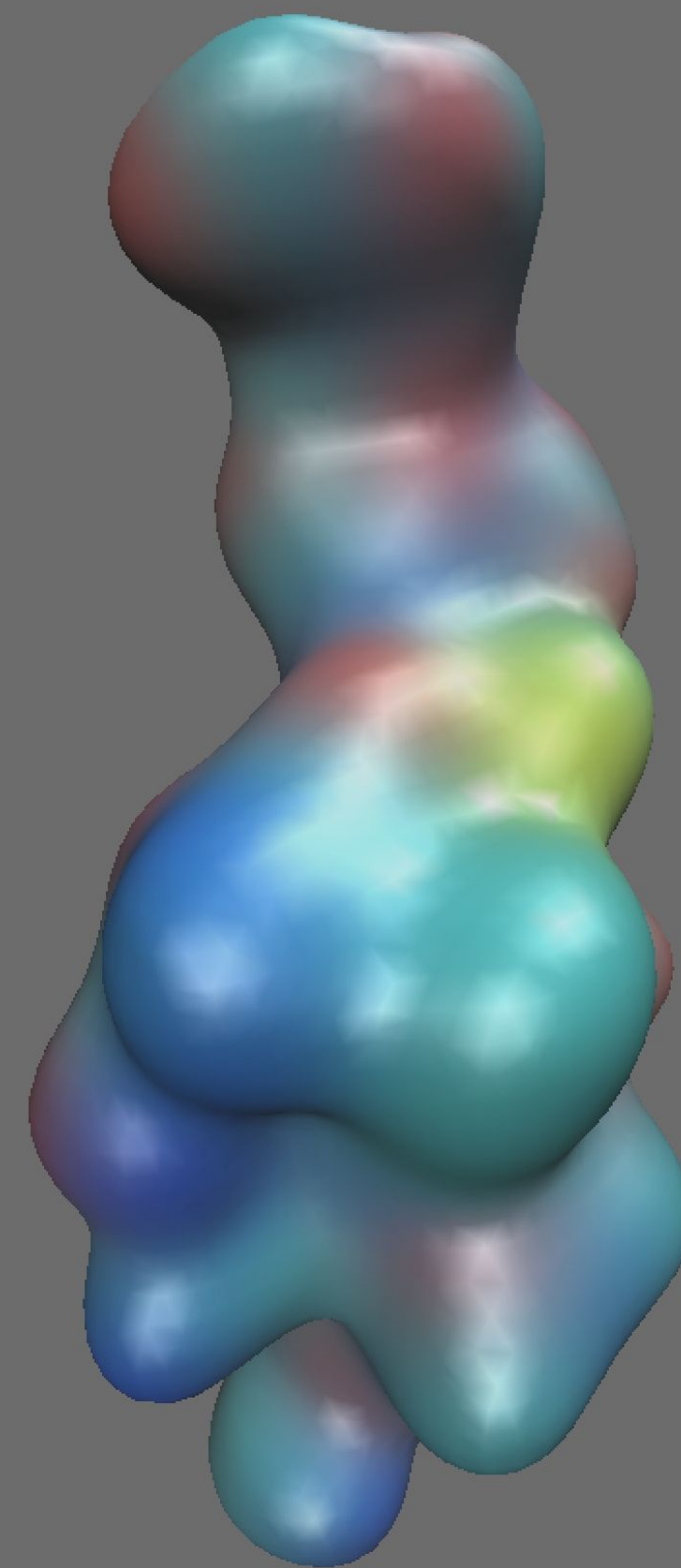
**Licorice:**  
Structure, atoms.  
Minimalistic.  
Looks better.



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



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



**Quick Surf:**  
Volume.  
Clean.



VMD Main

File Molecule Graphics Display Mouse

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

0 | 100

zoom ☐ Loop  1 speed

Graphical Representations

Selected Molecule

0: peptide.pdb

Create Rep Delete Rep

Style	Color	Selection
NewCartoon	Structure	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

Coloring Method: Secondary Stri

Drawing Method: NewCartoon

Material: Opaque

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 →

alpha-Helix →

Coil →

Coil

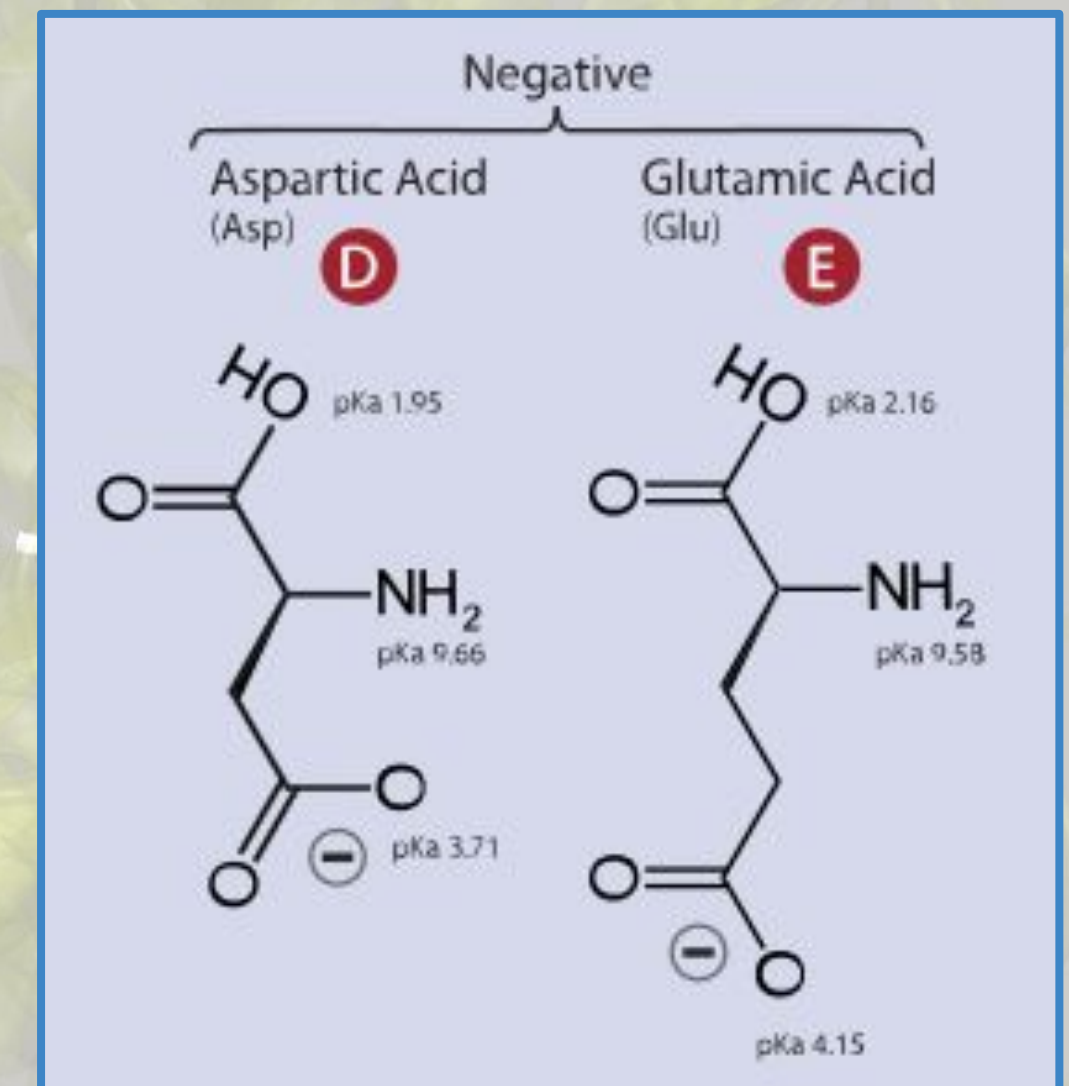
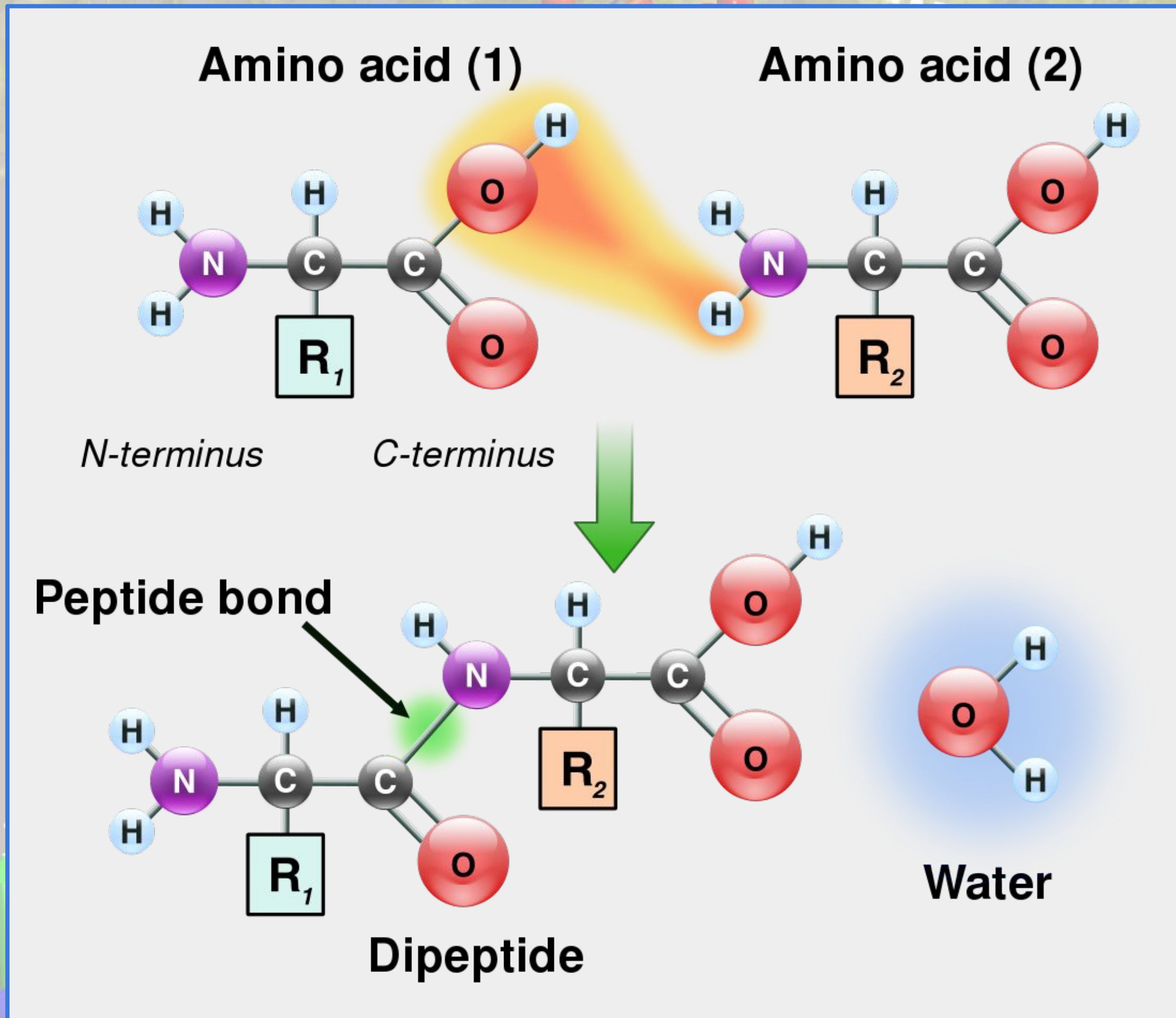
**NewCartoon:**  
Secondary structure based method.  
Highlights structural motifs.  
Removes atomistic details.

**Secondary Structure** coloring.

**Drawing methods**



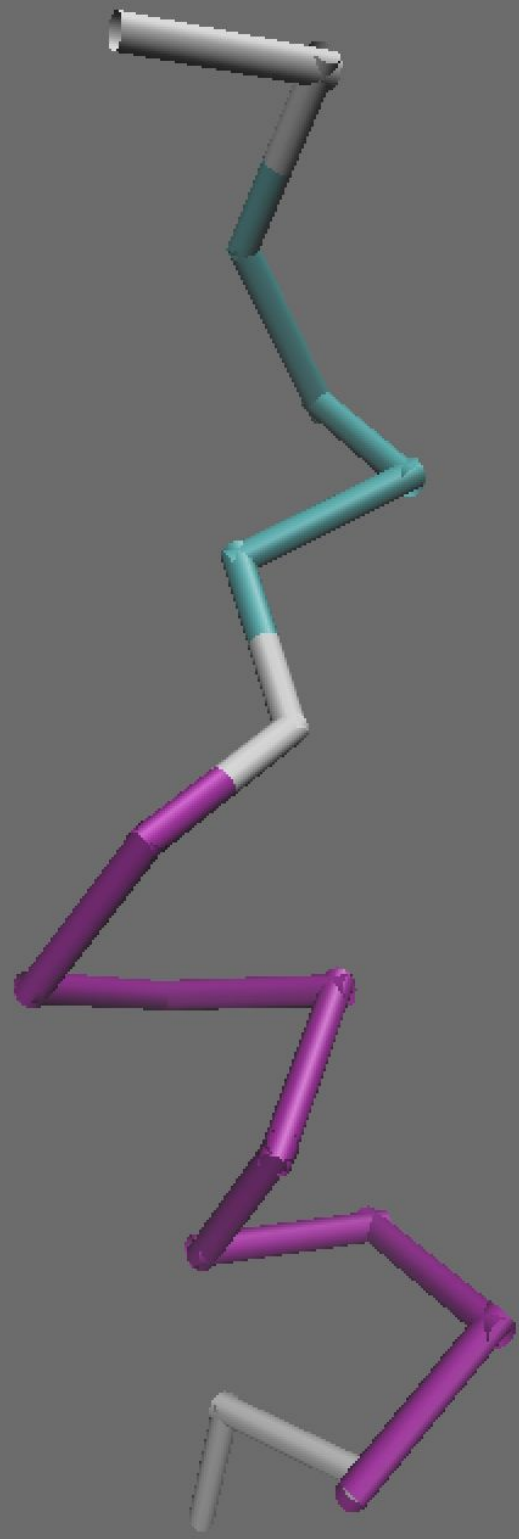
# Peptide bonds and peptides



- **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**:  $[C-C-N]_n$ .
- Most common: **alpha-helices** and **beta-sheets**.



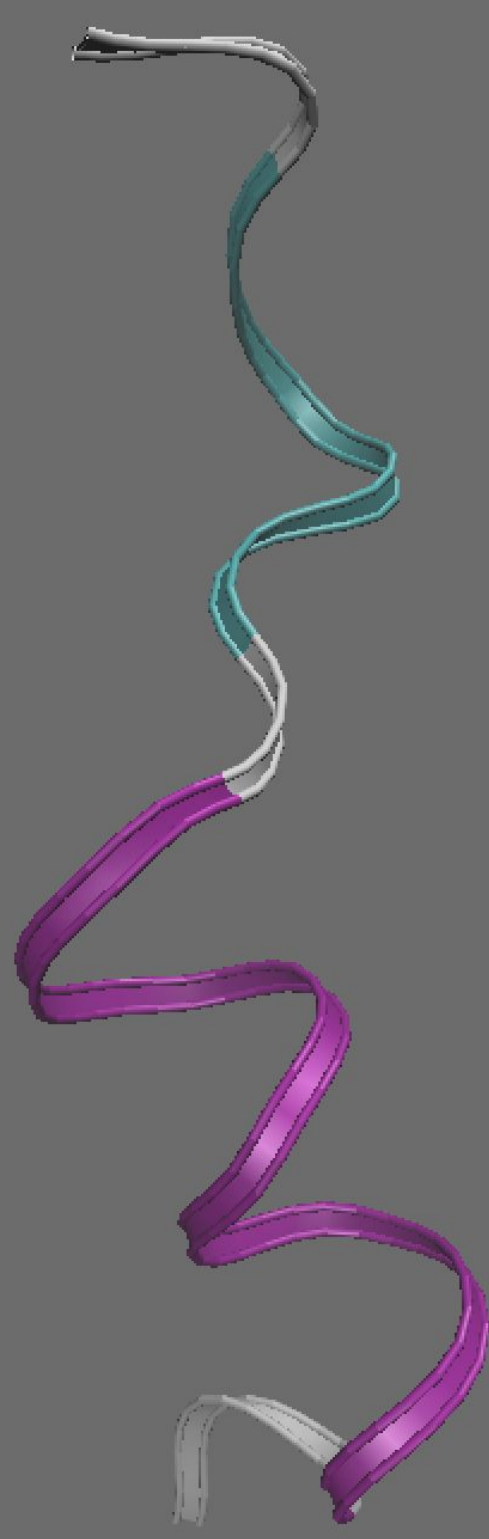
# Secondary Structure based Drawing Methods



**Trace:**  
Peptide  
backbone  
information.



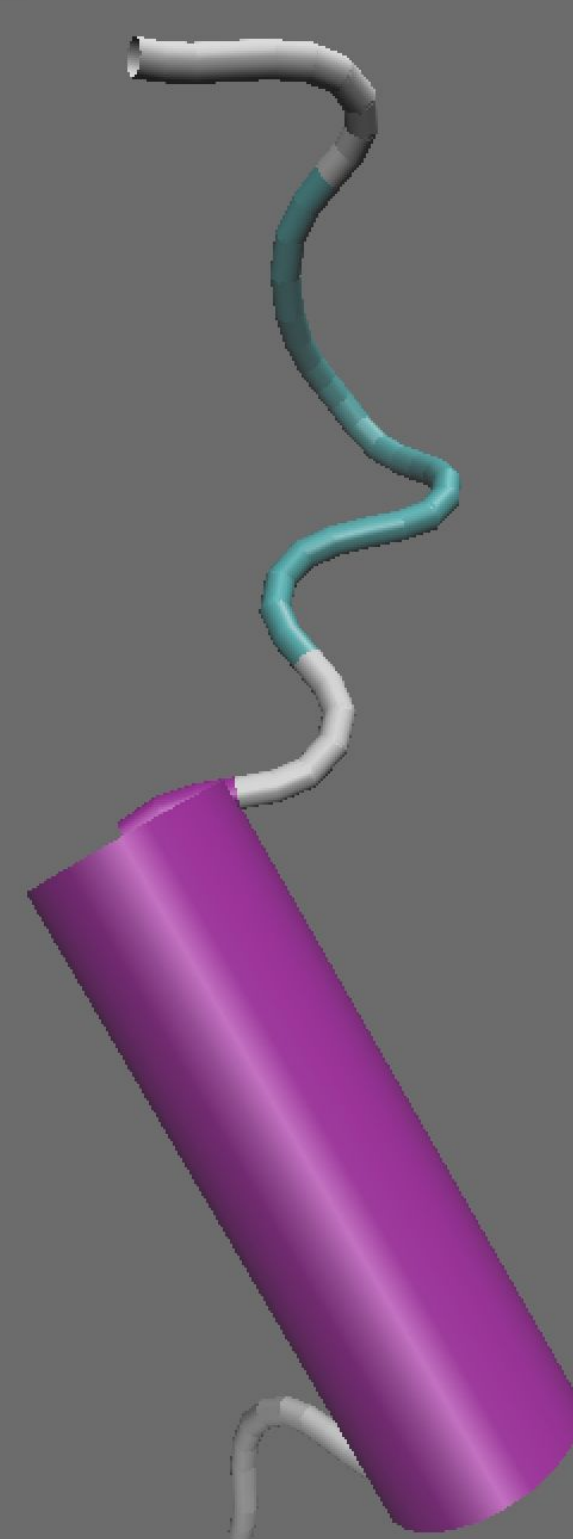
**Tube:**  
Smoothed  
backbone.  
Looks much  
cleaner.



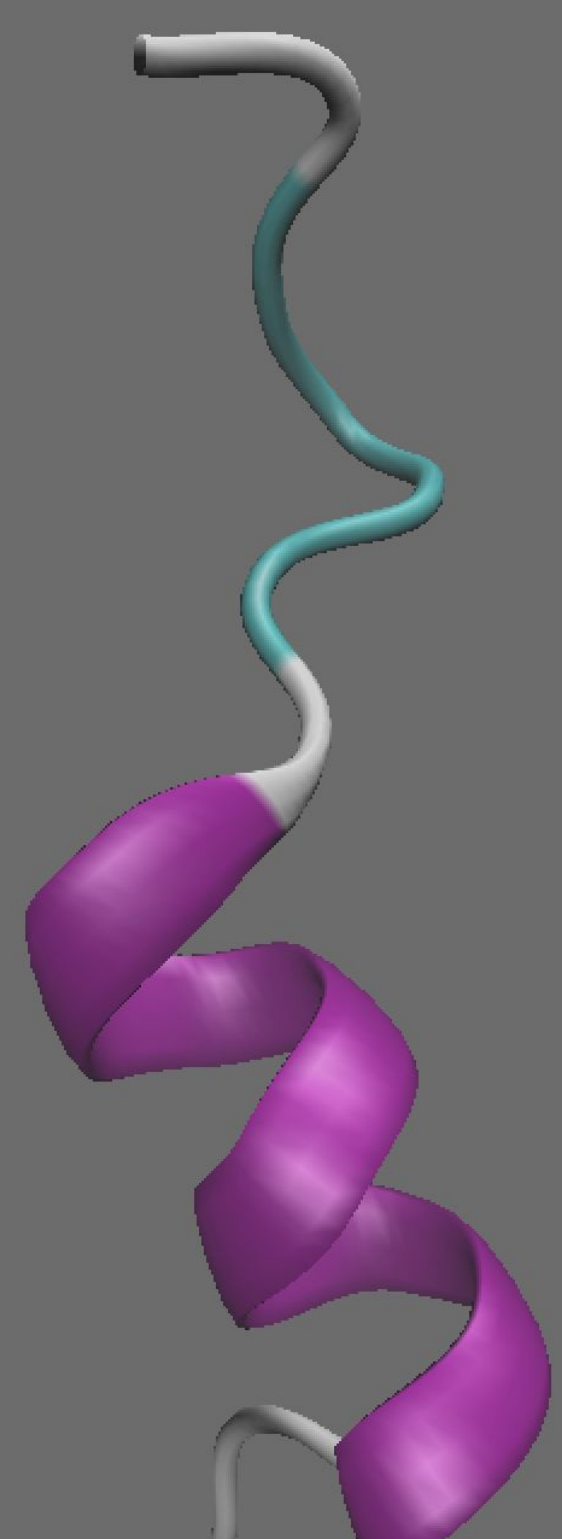
**Ribbons:**  
Backbone  
orientation  
information



**NewRibbons:**  
Cleaner new  
version.



**Cartoon:**  
Backbone with  
Secondary motif  
assignments.



**NewCartoon:**  
Cleaner new  
version.



VMD Main

File Molecule Graphics Display Mouse

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

0 | [Slider]

zoom [ ] Loop [v] step [1] speed [ ]

Graphical Representations

Selected Molecule

0: speptide.pdb [v]

Create Rep Delete Rep

Style	Color	Selection
VDW	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic |

Coloring Method [Name v]

Material [Opaque v]

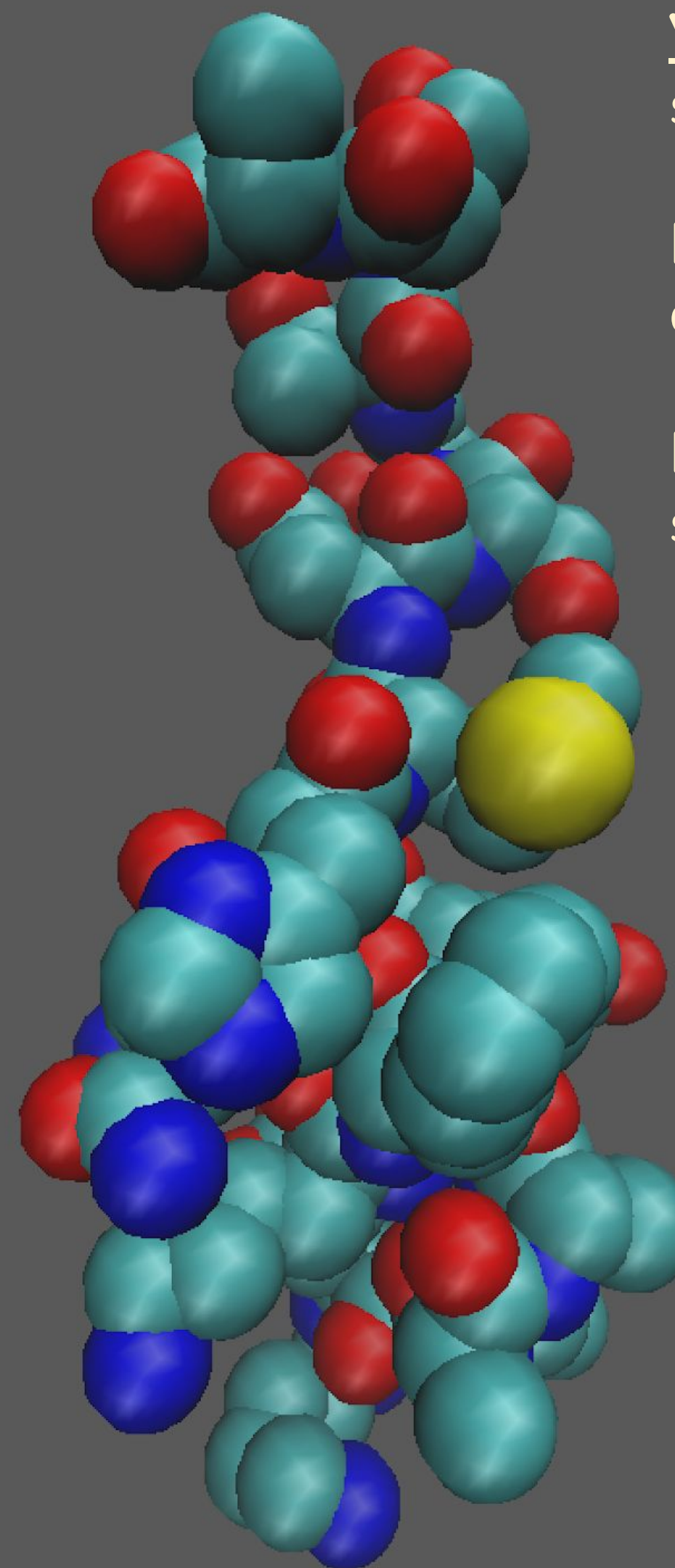
Drawing Method [VDW v]

Default

Sphere Scale [1.0]

Sphere Resolution [12]

Apply Changes Automatically [Apply]



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



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

# Screen Projection



**VMD Main**

File Molecule Graphics **Display** Mouse Extensions Help

ID	T	A	D	F	Molecule	Reset View	Frames	Vol
0	T	A	D	F	speptide.pdb	Stop Rotation	1	0

☐ Perspective  
☒ Orthographic  
☐ Antialiasing  
☒ **Depth Cueing**  
☐ Culling  
☐ FPS Indicator

Light settings:  
☒ Light 0  
☒ Light 1  
☐ Light 2  
☐ Light 3

Selected Mole: 0: speptide.pdb

Create Rep

Style	Color
VDW	Name

Selected Atoms: all

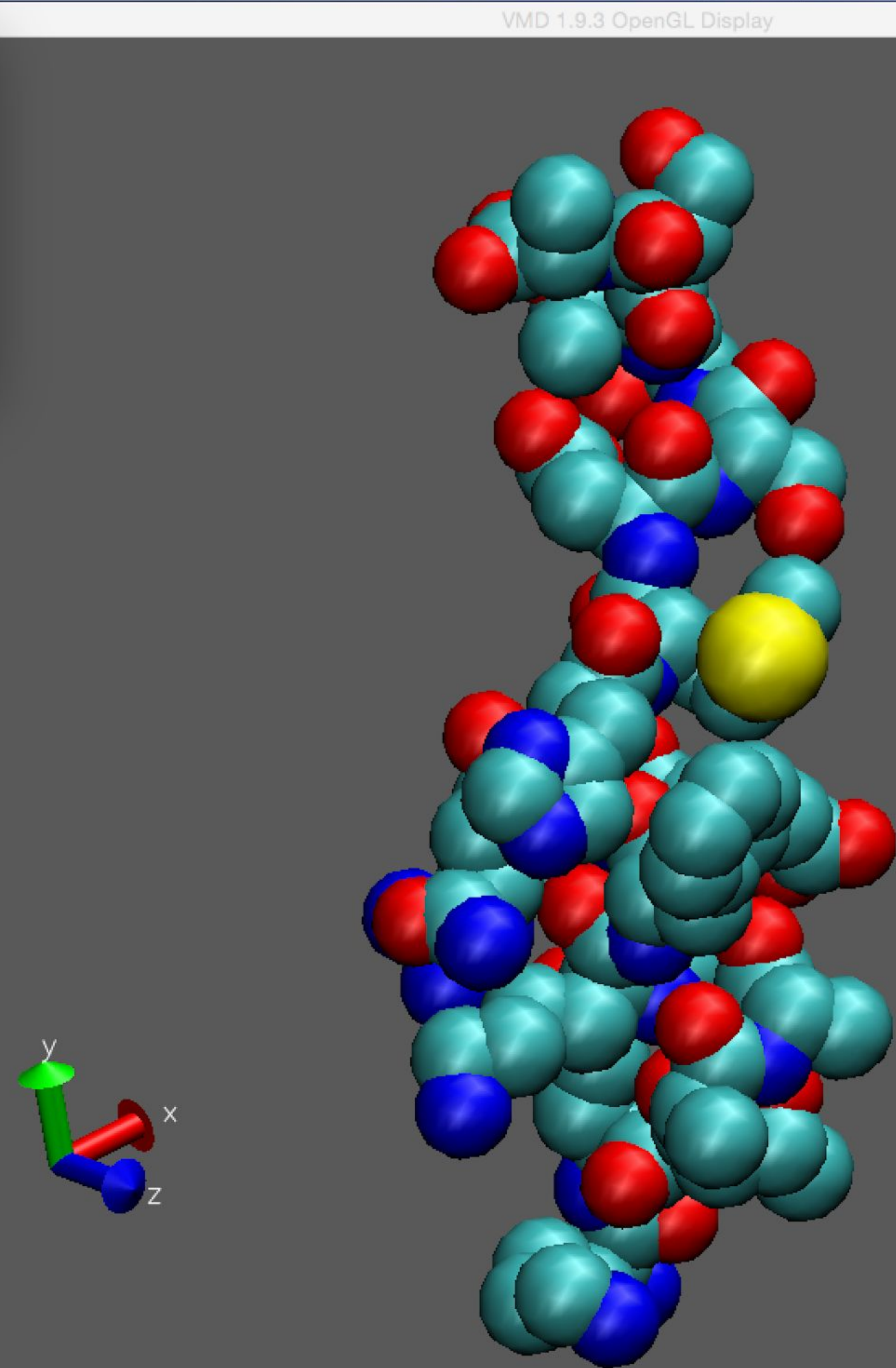
Draw style: Selections Trajectory Periodic

Coloring Method: Name Material: Opaque

Drawing Method: VDW Default

Sphere Scale: 1.0  
Sphere Resolution: 12

Apply Changes Automatically Apply



## Depth Cueing:

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

# Depth Cueing



**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

Selected Mole: 0: peptide.pdb

Create Rep

Style	Color
VDW	Name

Selected Atoms: all

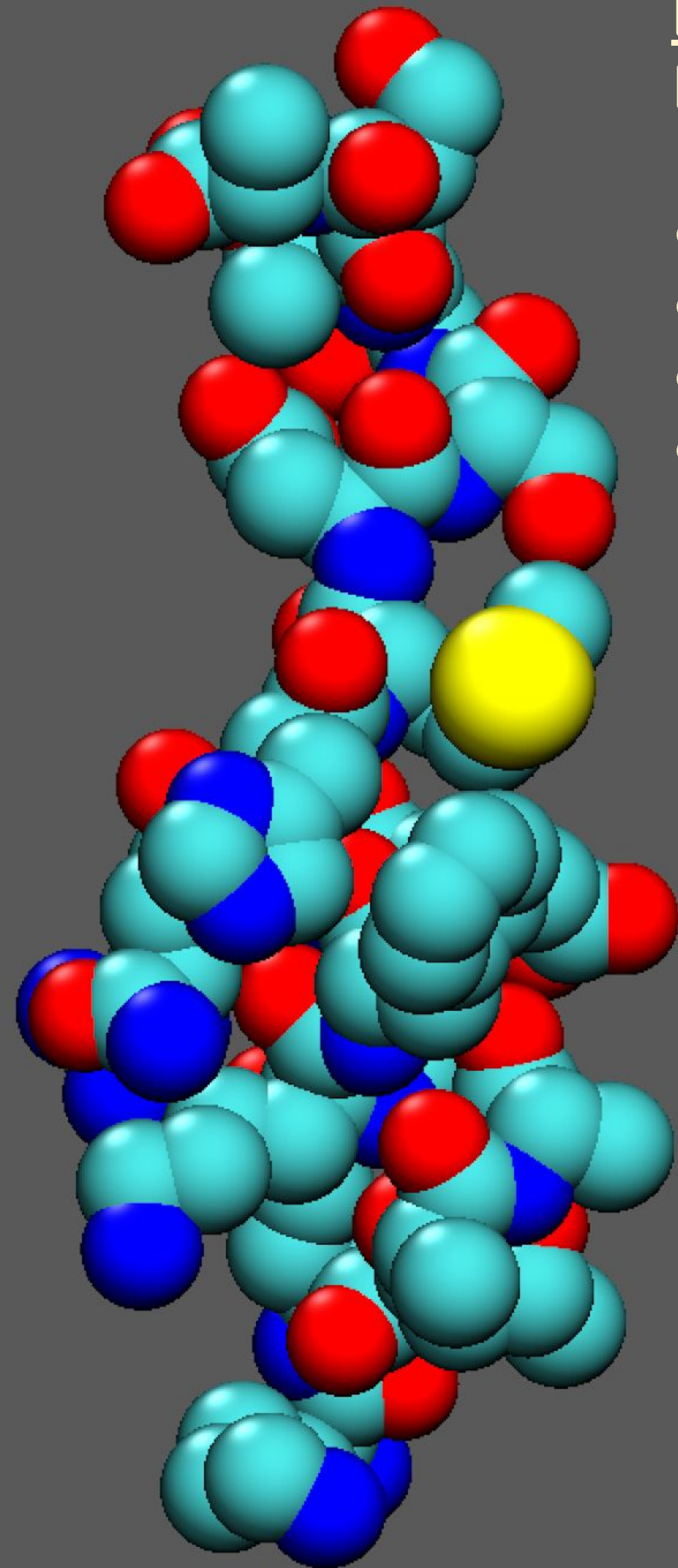
Draw style | Selections | Trajectory | Periodic |

Coloring Method: Name | Material: Opaque

Drawing Method: VDW | Default

Sphere Scale: 1.0 | Sphere Resolution: 12

Apply Changes Automatically | Apply



Rendermode GLSL:  
Hardware accelerated mode.

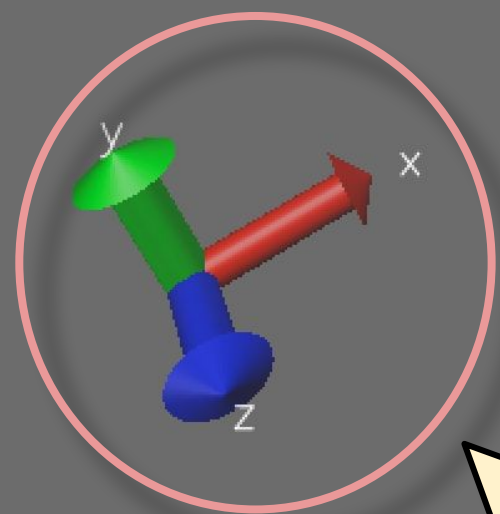
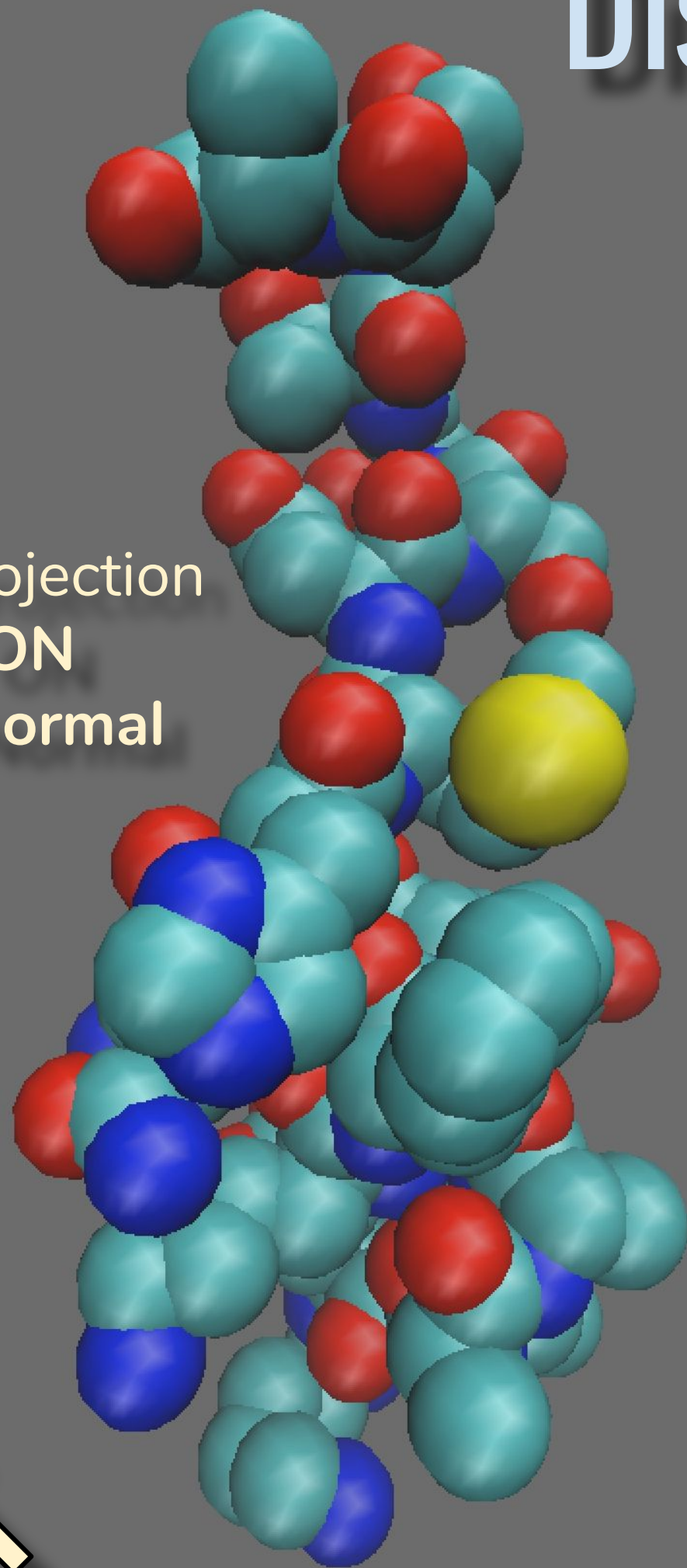
- Faster;
- Better looking;
- Needs a GPU video card.
- Much better for transparent materials.

# Rendermode

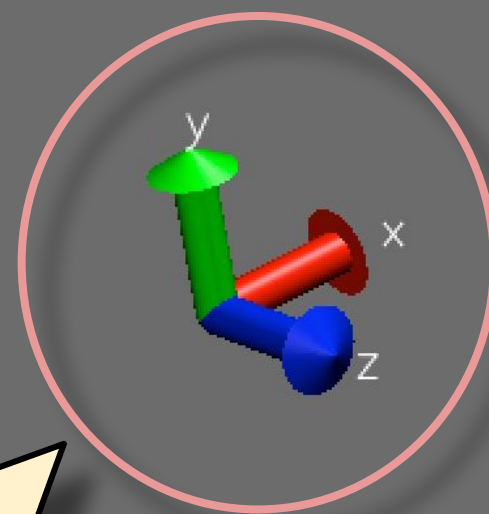
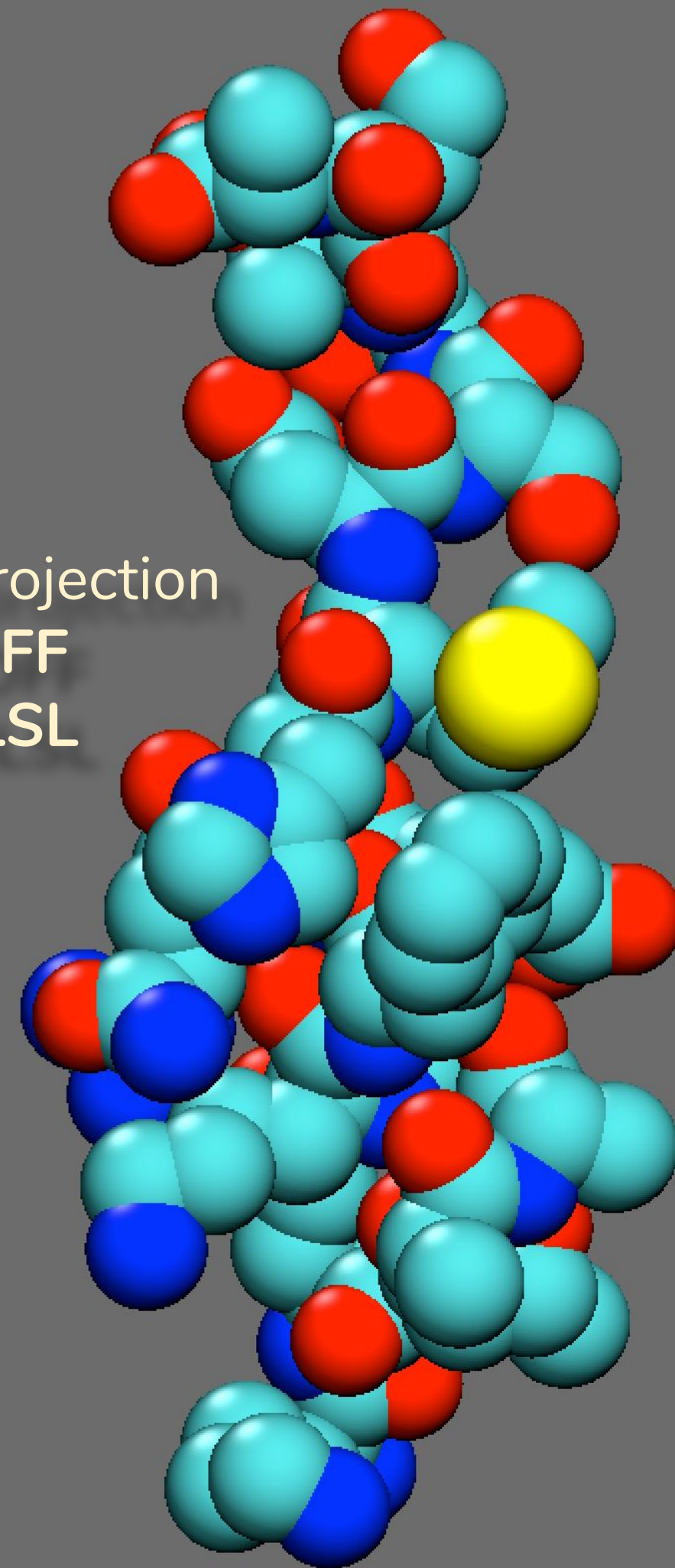


# Display modes

- **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 Main

File Molecule Graphics **Display** Mouse Extensions Help

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

Selected Mole  
0: speptide.pdb

Create Rep

Style Color  
Lines Name

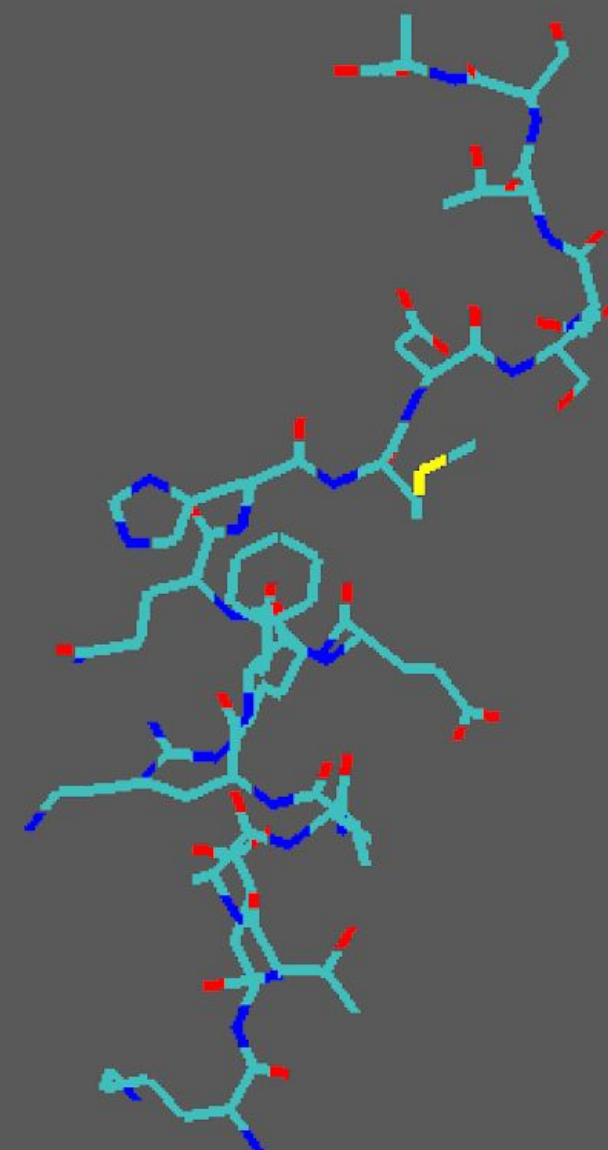
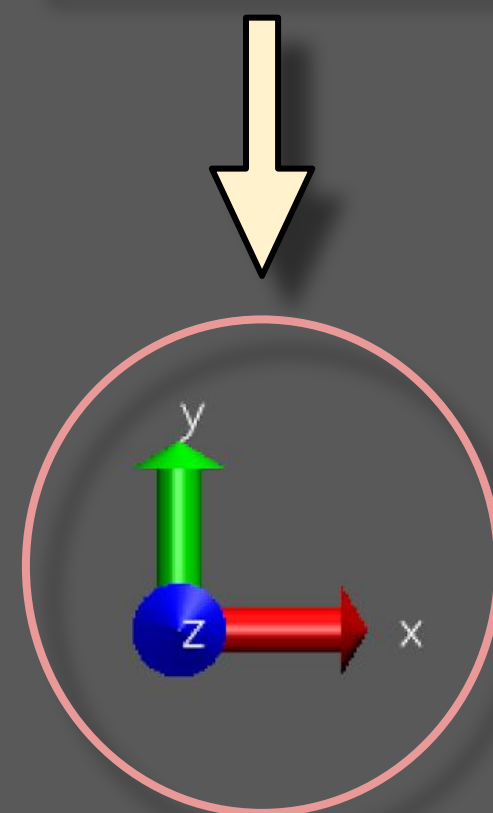
Selected Atoms  
all

Draw style | Selections | Trajectory | Periodic |  
Coloring Method Name Material Opaque  
Drawing Method Lines  
Thickness 4

Apply Changes Automatically Apply

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

Navigation controls: frame slider (0 to 1), zoom, Loop, step, speed.

Selected Molecule

2: peptide.pdb

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all

Selected Atoms

all

Draw style | Selections | Trajectory | Periodic

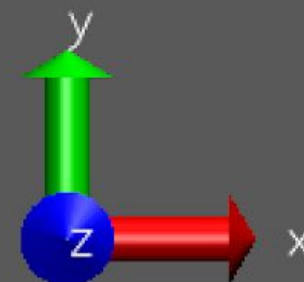
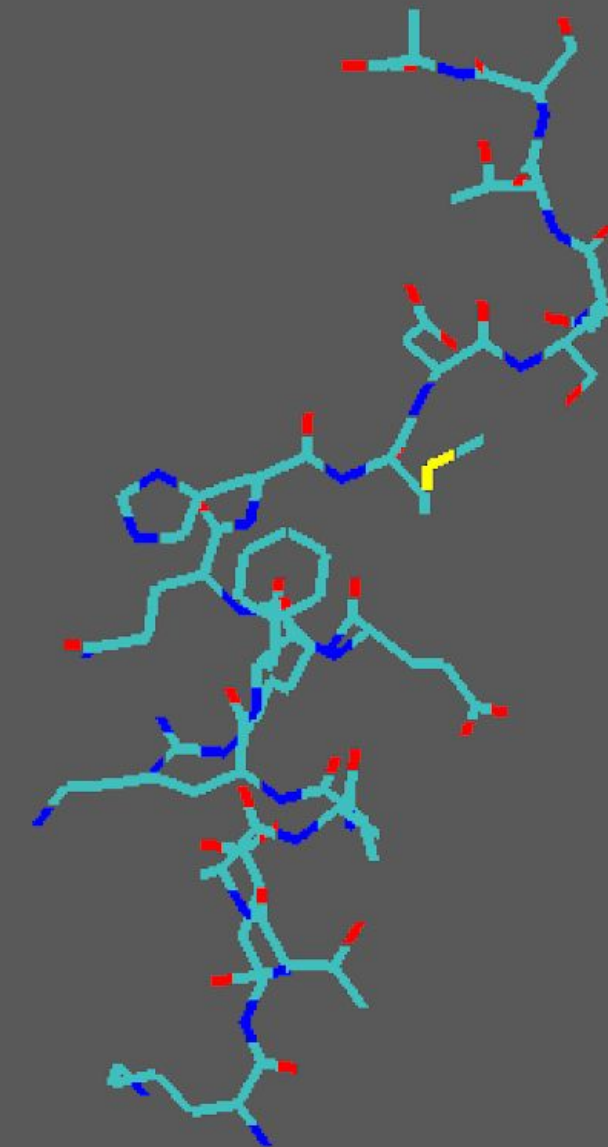
Coloring Method: Name Material: Opaque

Drawing Method: Lines Default

Thickness: 1

Apply Changes Automatically Apply

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



# Working on an illustration



VMD Main

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: peptide.pdb

?

Enter a new name for molecule 0:

peptide structure

OK

Cancel

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

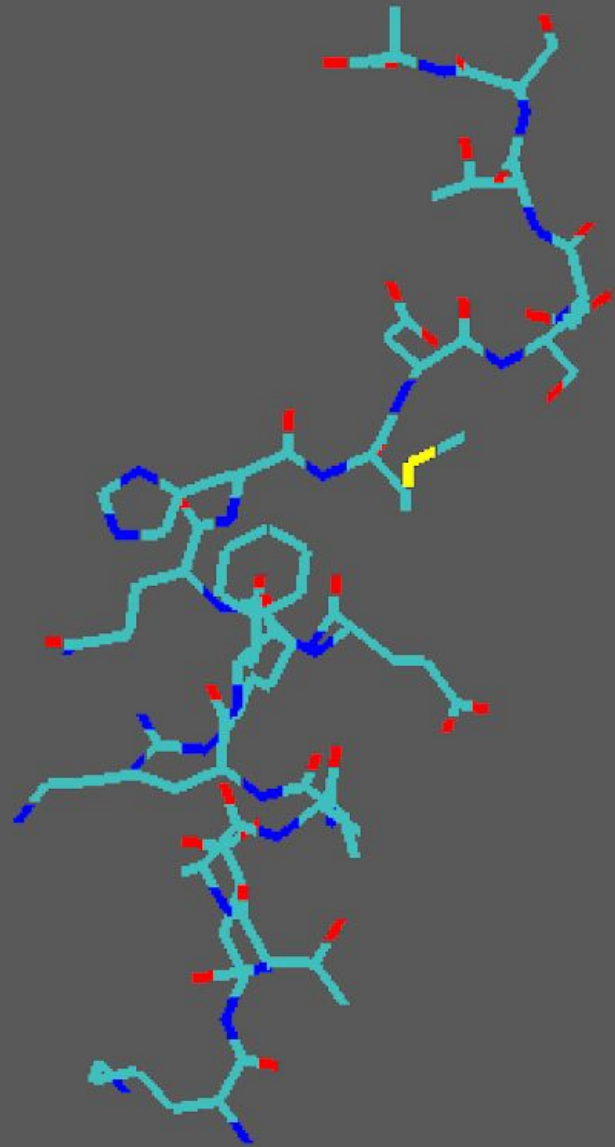
Thickness

1

Apply Changes Automatically

Apply

VMD 1.9.3 OpenGL Display



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

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

Timeline controls: frame 0, zoom, Loop, step 1, speed

Selected Molecule: 2: peptide volume

Create Rep Delete Rep

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Draw style | Selections | Trajectory | Periodic

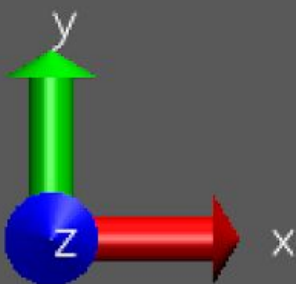
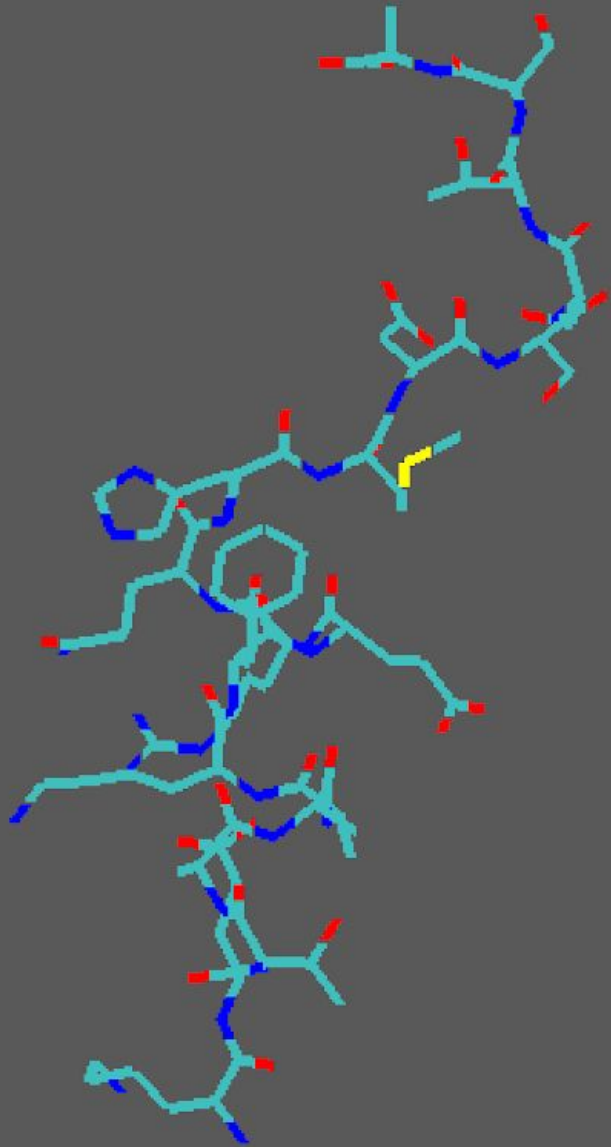
Coloring Method: Name Material: Opaque

Drawing Method: Lines Default

Thickness: 1

Apply Changes Automatically Apply

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



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

0 [Timeline bar]

zoom [checkbox] Loop [dropdown] step 1 speed [slider]

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

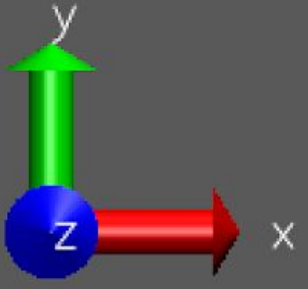
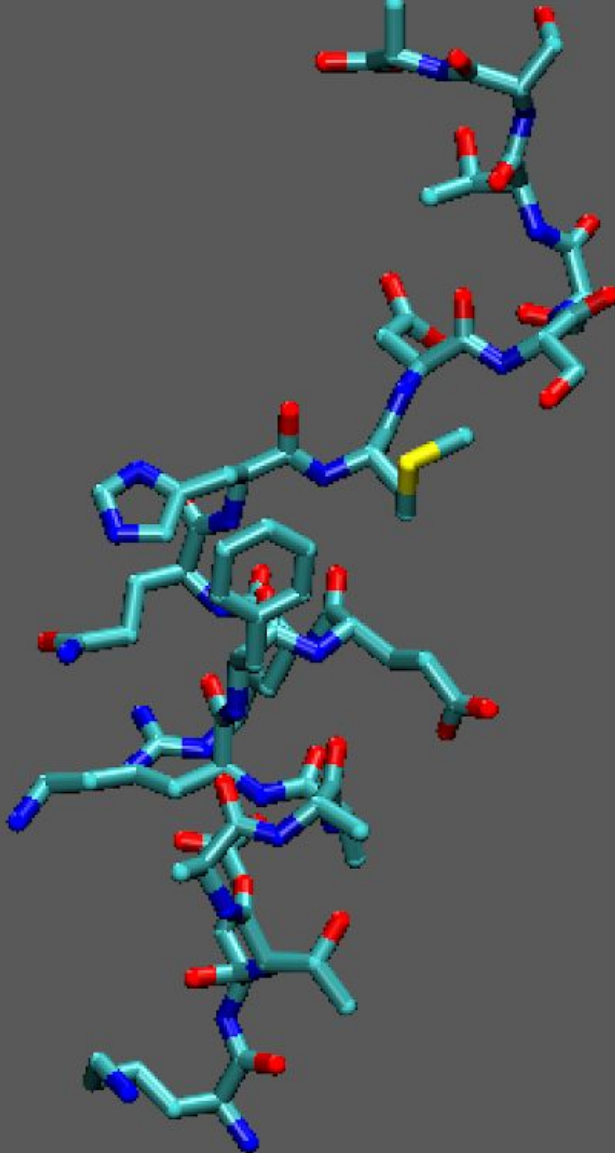
Drawing Method: Licorice

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 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

0: speptide structure

Mouse menu:

- ☒ Rotate Mode
- ☐ Translate Mode
- ☐ Scale Mode
- ☐ Center
- ☐ Query
- ☐ Label
- ☒ **Move**
  - ☐ Atom 5
  - ☐ Residue 6
  - ☐ Fragment 7
  - ☒ **Molecule 8**
  - ☐ Rep 9
- ☐ Force
- ☐ Move Light
- ☐ Add/Remove Bonds
- ☐ Pick

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

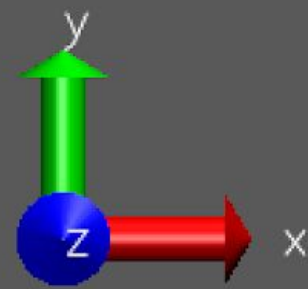
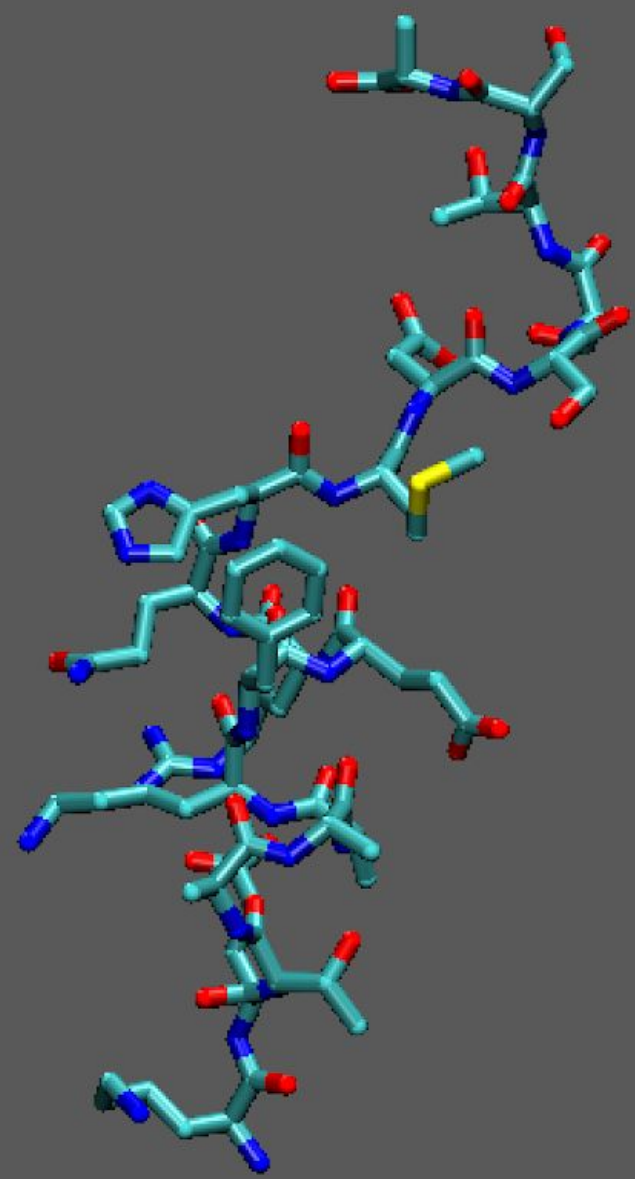
Drawing Method: Licorice Default

Sphere Resolution: 12

Bond Radius: 0.3

Bond Resolution: 12

Apply Changes Automatically Apply

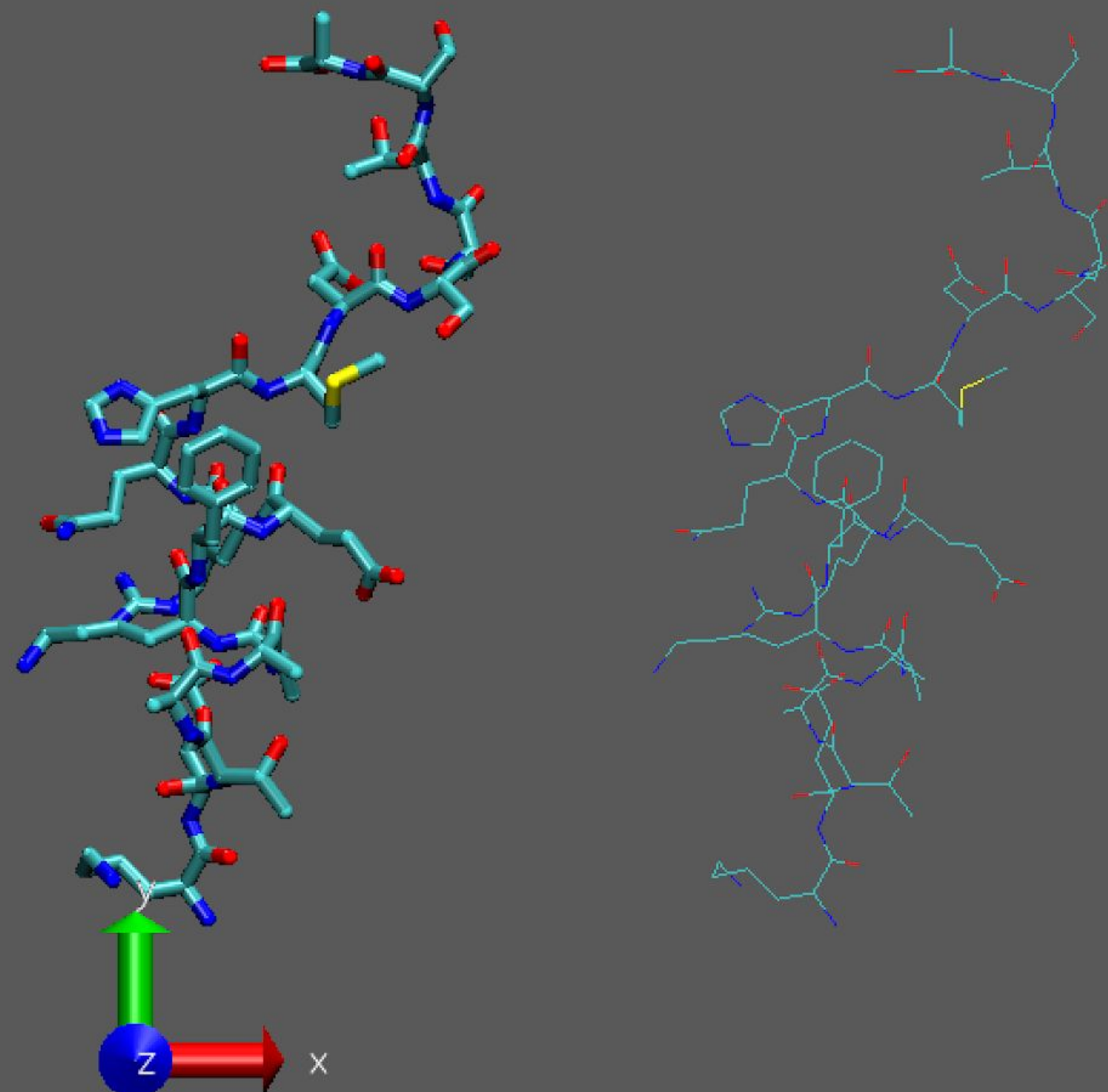


- Change the mouse mode to **Move Molecule**.

Working on an illustration



- 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 [Slider] [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

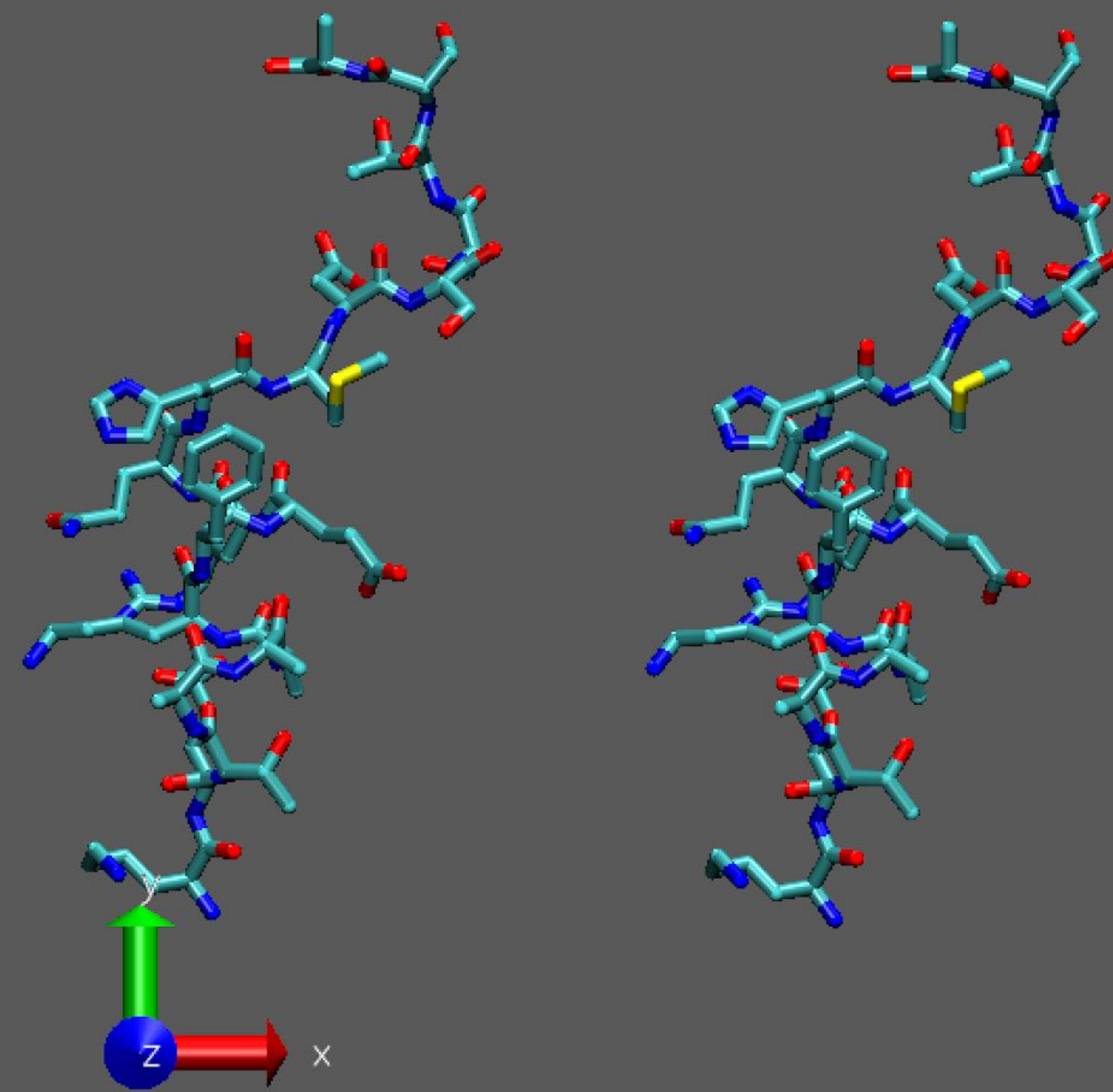
Coloring Method: Name Material: Opaque

Drawing Method: Licorice

Sphere Resolution: 12 Bond Radius: 0.3 Bond Resolution: 12

Apply Changes Automatically Apply

- Repeat with the “volume” molecule.



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 [Timeline bar] zoom [ ] Loop [v] step [1] speed [ ]

Graphical Representations

Selected Molecule

2: speptide volume

Create Rep Delete Rep

Style	Color	Selection
Licorice	Name	all

Selected Atoms

all

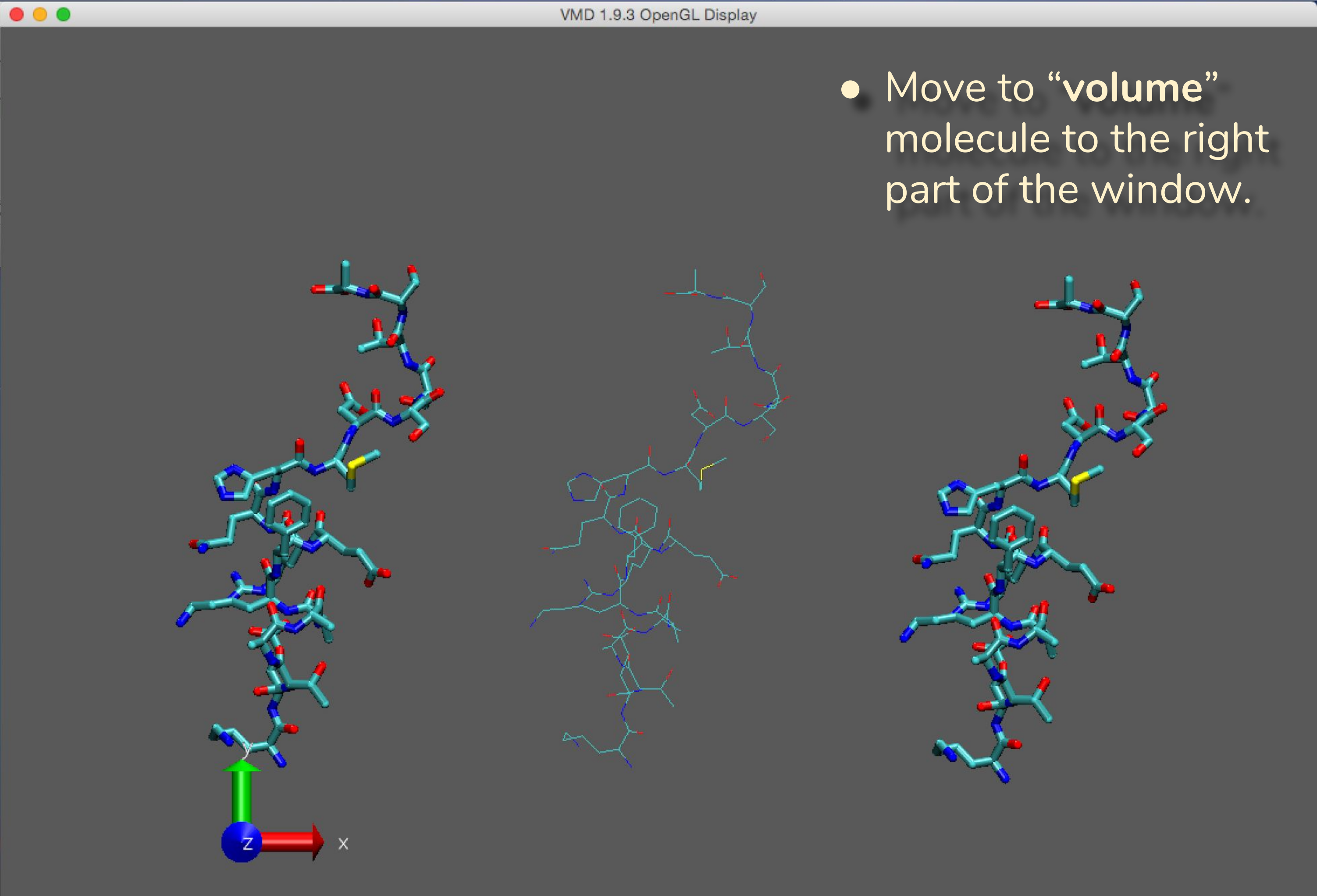
Draw style | Selections | Trajectory | Periodic

Coloring Method: Name Material: Opaque

Drawing Method: Licorice Default

Sphere Resolution: 12 Bond Radius: 0.3 Bond Resolution: 12

Apply Changes Automatically Apply



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

Working on an illustration



# 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 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301 302 303 304 305 306 307 308 309 310 311 312 313 314 315 316 317 318 319 320 321 322 323 324 325 326 327 328 329 330 331 332 333 334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359 360 361 362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387 388 389 390 391 392 393 394 395 396 397 398 399 400 401 402 403 404 405 406 407 408 409 410 411 412 413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432 433 434 435 436 437 438 439 440 441 442 443 444 445 446 447 448 449 450 451 452 453 454 455 456 457 458 459 460 461 462 463 464 465 466 467 468 469 470 471 472 473 474 475 476 477 478 479 480 481 482 483 484 485 486 487 488 489 490 491 492 493 494 495 496 497 498 499 500 501 502 503 504 505 506 507 508 509 510 511 512 513 514 515 516 517 518 519 520 521 522 523 524 525 526 527 528 529 530 531 532 533 534 535 536 537 538 539 540 541 542 543 544 545 546 547 548 549 550 551 552 553 554 555 556 557 558 559 560 561 562 563 564 565 566 567 568 569 570 571 572 573 574 575 576 577 578 579 580 581 582 583 584 585 586 587 588 589 590 591 592 593 594 595 596 597 598 599 600 601 602 603 604 605 606 607 608 609 610 611 612 613 614 615 616 617 618 619 620 621 622 623 624 625 626 627 628 629 630 631 632 633 634 635 636 637 638 639 640 641 642 643 644 645 646 647 648 649 650 651 652 653 654 655 656 657 658 659 660 661 662 663 664 665 666 667 668 669 670 671 672 673 674 675 676 677 678 679 680 681 682 683 684 685 686 687 688 689 690 691 692 693 694 695 696 697 698 699 700 701 702 703 704 705 706 707 708 709 710 711 712 713 714 715 716 717 718 719 720 721 722 723 724 725 726 727 728 729 730 731 732 733 734 735 736 737 738 739 740 741 742 743 744 745 746 747 748 749 750 751 752 753 754 755 756 757 758 759 760 761 762 763 764 765 766 767 768 769 770 771 772 773 774 775 776 777 778 779 780 781 782 783 784 785 786 787 788 789 790 791 792 793 794 795 796 797 798 799 800 801 802 803 804 805 806 807 808 809 810 811 812 813 814 815 816 817 818 819 820 821 822 823 824 825 826 827 828 829 830 831 832 833 834 835 836 837 838 839 840 841 842 843 844 845 846 847 848 849 850 851 852 853 854 855 856 857 858 859 860 861 862 863 864 865 866 867 868 869 870 871 872 873 874 875 876 877 878 879 880 881 882 883 884 885 886 887 888 889 890 891 892 893 894 895 896 897 898 899 900 901 902 903 904 905 906 907 908 909 910 911 912 913 914 915 916 917 918 919 920 921 922 923 924 925 926 927 928 929 930 931 932 933 934 935 936 937 938 939 940 941 942 943 944 945 946 947 948 949 950 951 952 953 954 955 956 957 958 959 960 961 962 963 964 965 966 967 968 969 970 971 972 973 974 975 976 977 978 979 980 981 982 983 984 985 986 987 988 989 990 991 992 993 994 995 996 997 998 999 1000

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 Str

Drawing Method

NewCartoon

Material

Opaque

Default

Spline Style

Catmull-Rom

Aspect Ratio

4.10

Thickness

0.30

Resolution

10

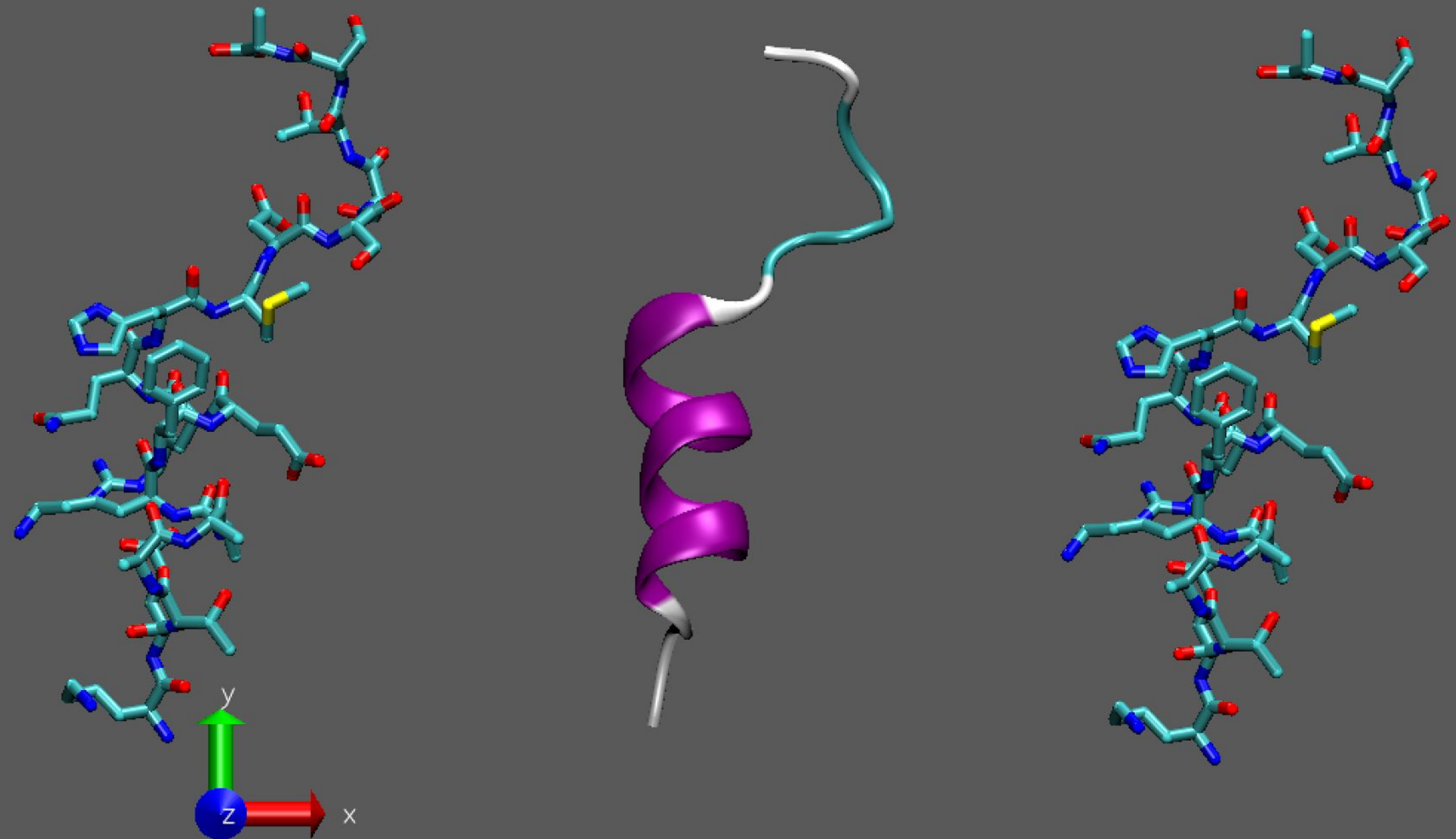
Apply Changes Automatically Apply

In Representations window:

- Select the “cartoon” molecule;

- Drawing method: **NewCartoon**;

- Coloring: **Secondary Structure**.



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
QuickSurf	Name	all

Selected Atoms

all

Draw style

Selections

Trajectory

Periodic

Coloring Method

Name

Drawing Method

QuickSurf

Material

Opaque

Resolution

0.50

Radius Scale

0.5

Density Isovalue

0.5

Grid Spacing

0.2

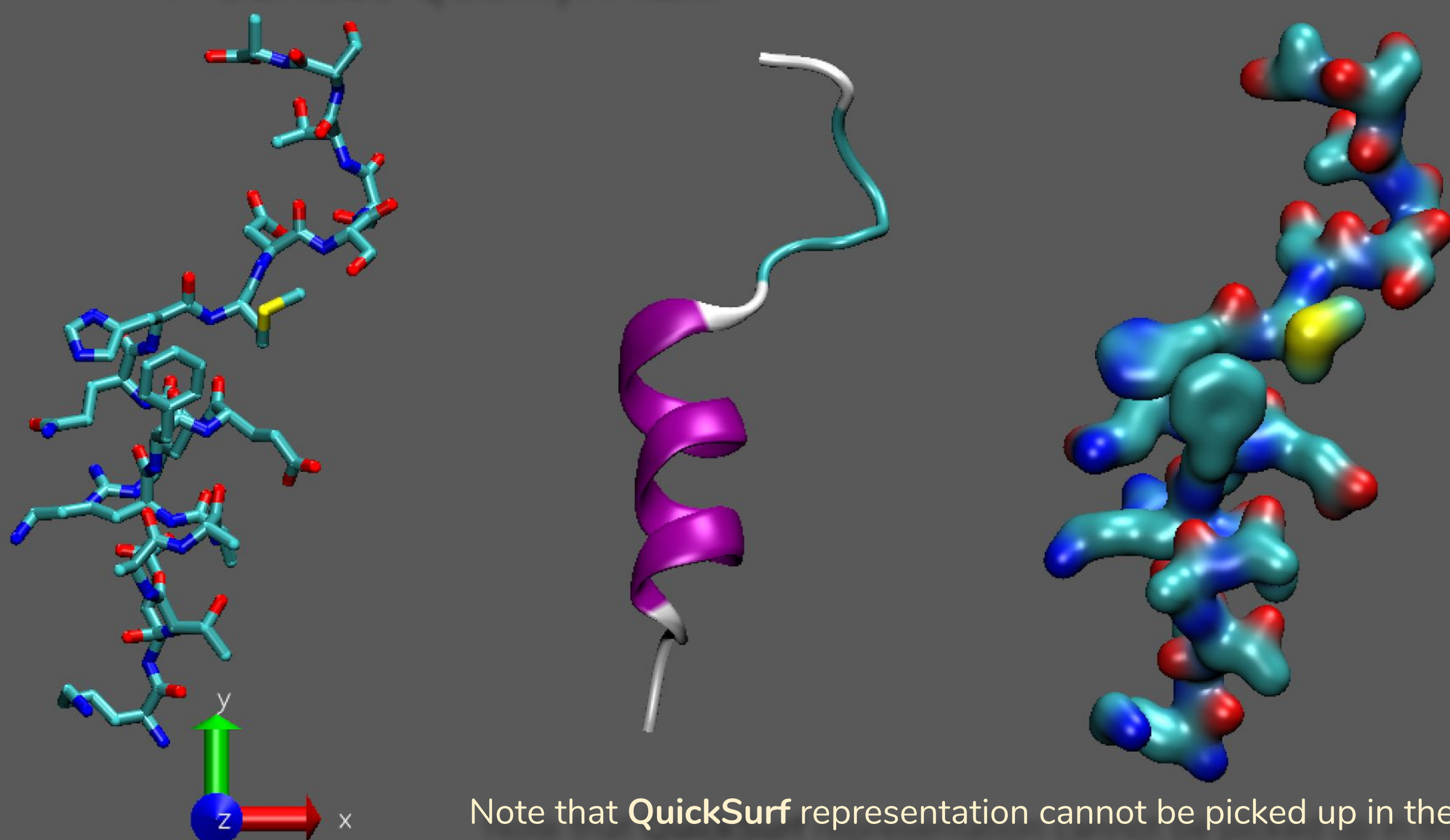
Surface Quality

Max

Apply Changes Automatically

Apply

- 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

Reset View =

Stop Rotation

☐ Perspective

☒ Orthographic

☐ Antialiasing

☐ Depth Cueing

☐ Culling

☐ FPS Indicator

☒ Light 0

☒ Light 1

☐ Light 2

☐ Light 3

**Axes**

☐ Off

☐ Origin

☐ LowerLeft

☐ LowerRight

☒ UpperLeft

☐ UpperRight

Background

Stage

Stereo

Stereo Eye Swap

Cachemode

Rendermode

Display Settings...

Selected Mole

2: peptide 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

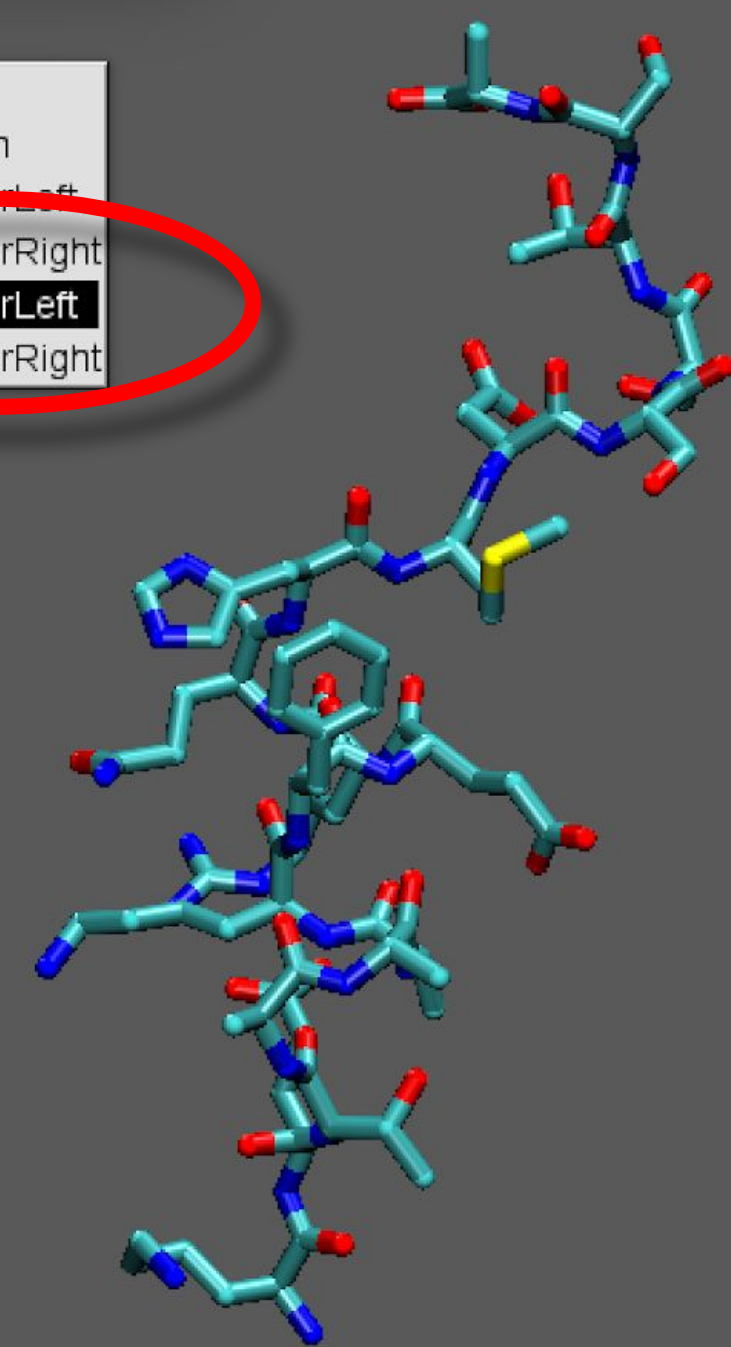
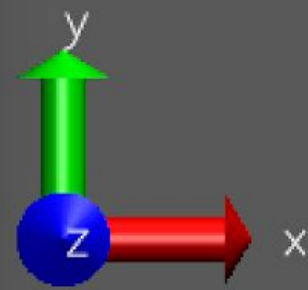
Density Isovalue 0.5

Grid Spacing 0.2

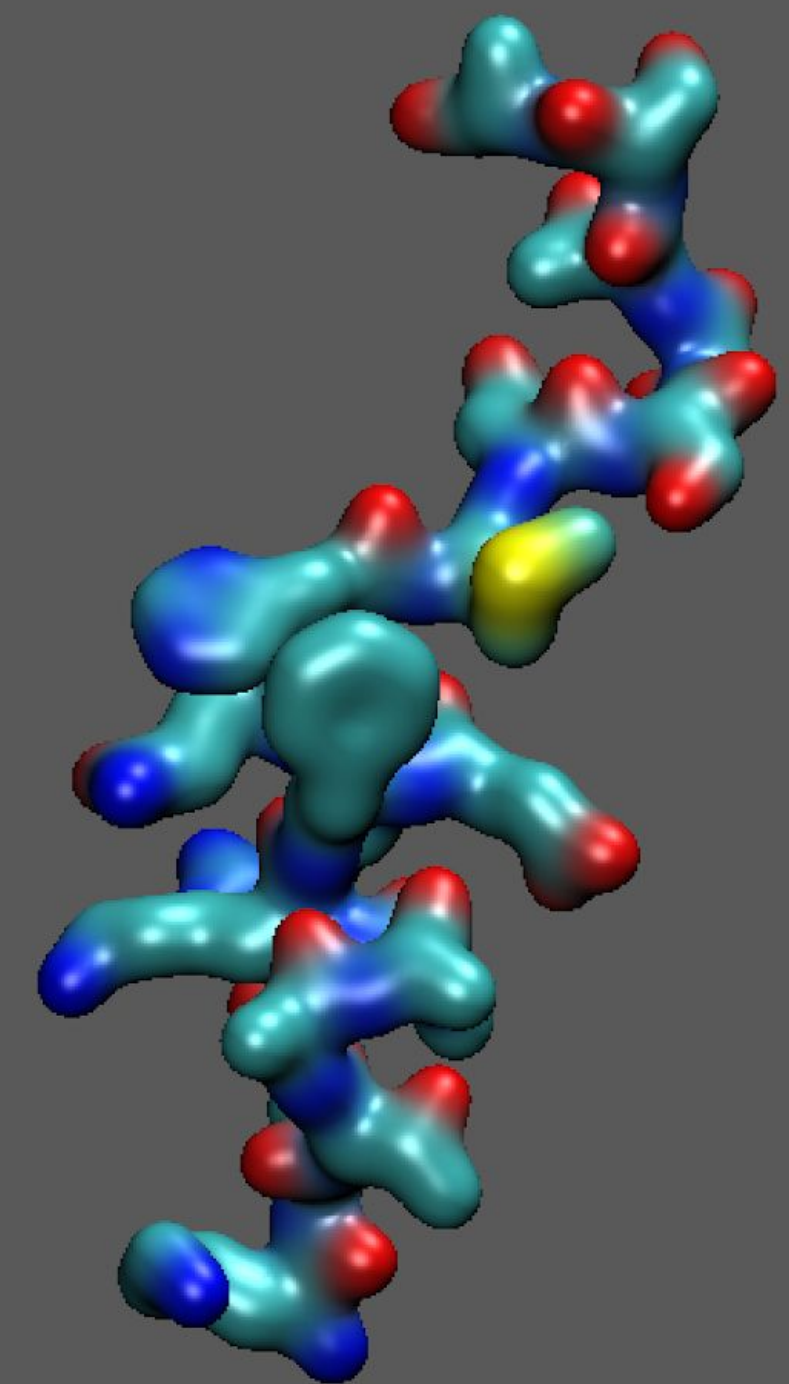
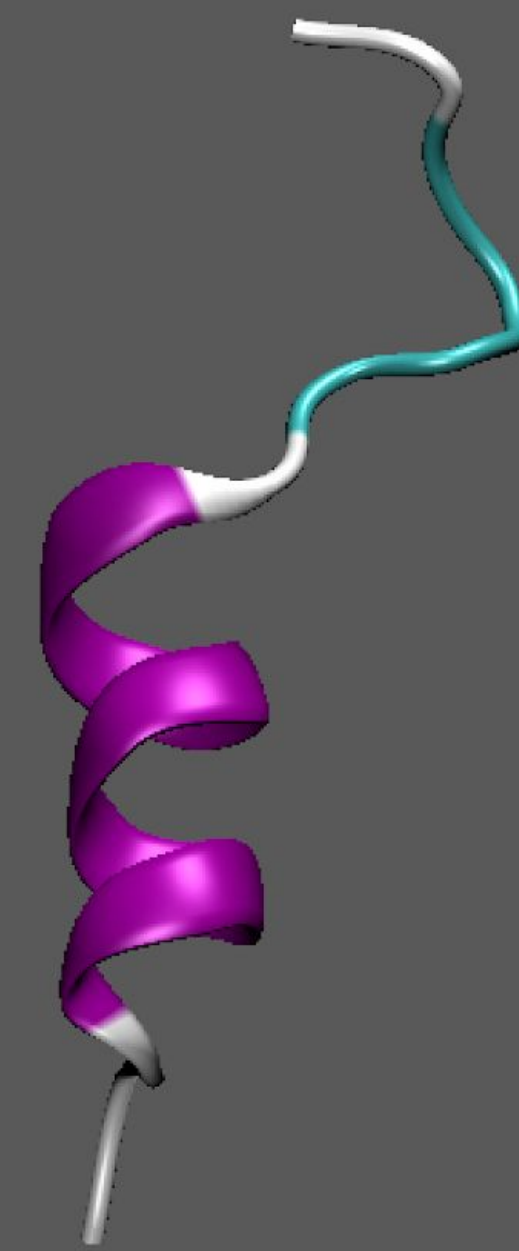
Surface Quality Max

Apply Changes Automatically

Apply



- 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

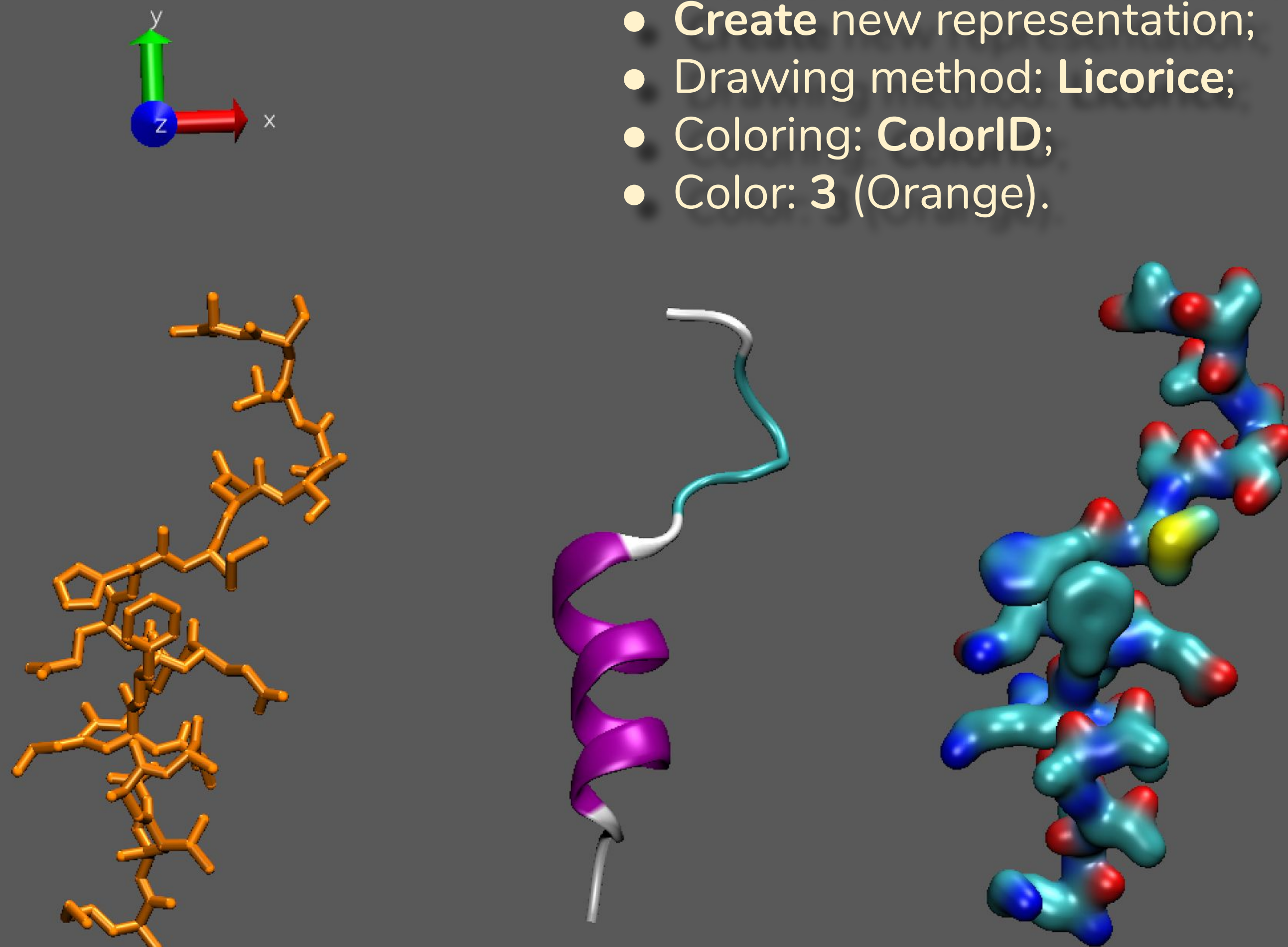
Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Apply Changes Automatically Apply

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



# 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   [slider]   zoom   [checkbox]   Loop   [dropdown]   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

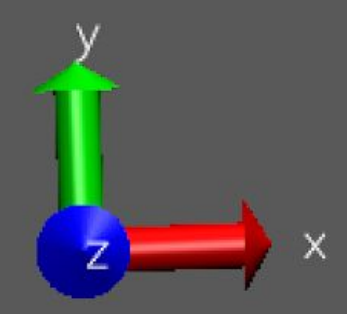
and   or   not

Apply   Reset

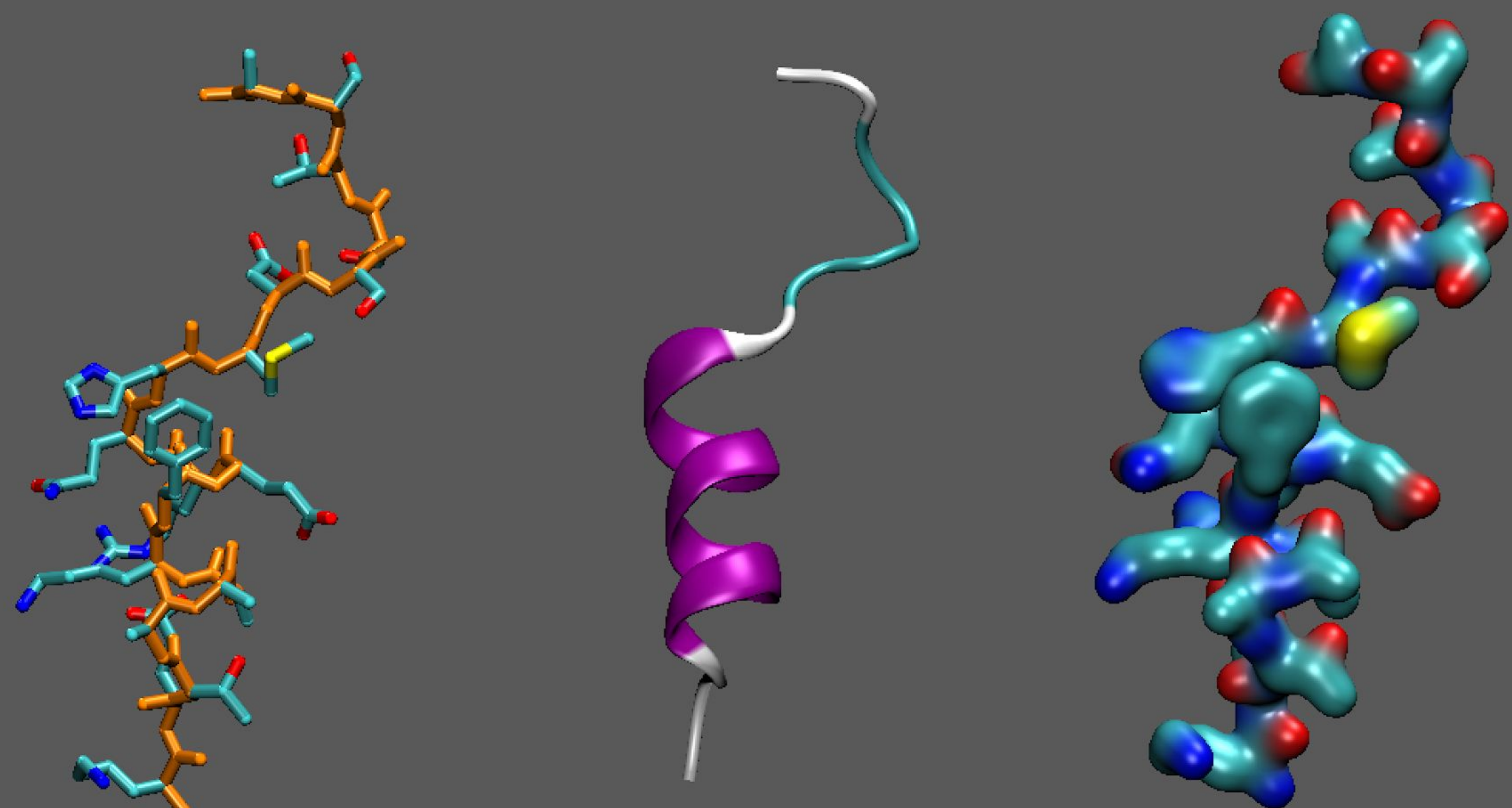
Macro definition:

alpha\_helix

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



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



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

1: peptide cartoon

Create Rep Delete Rep

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

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

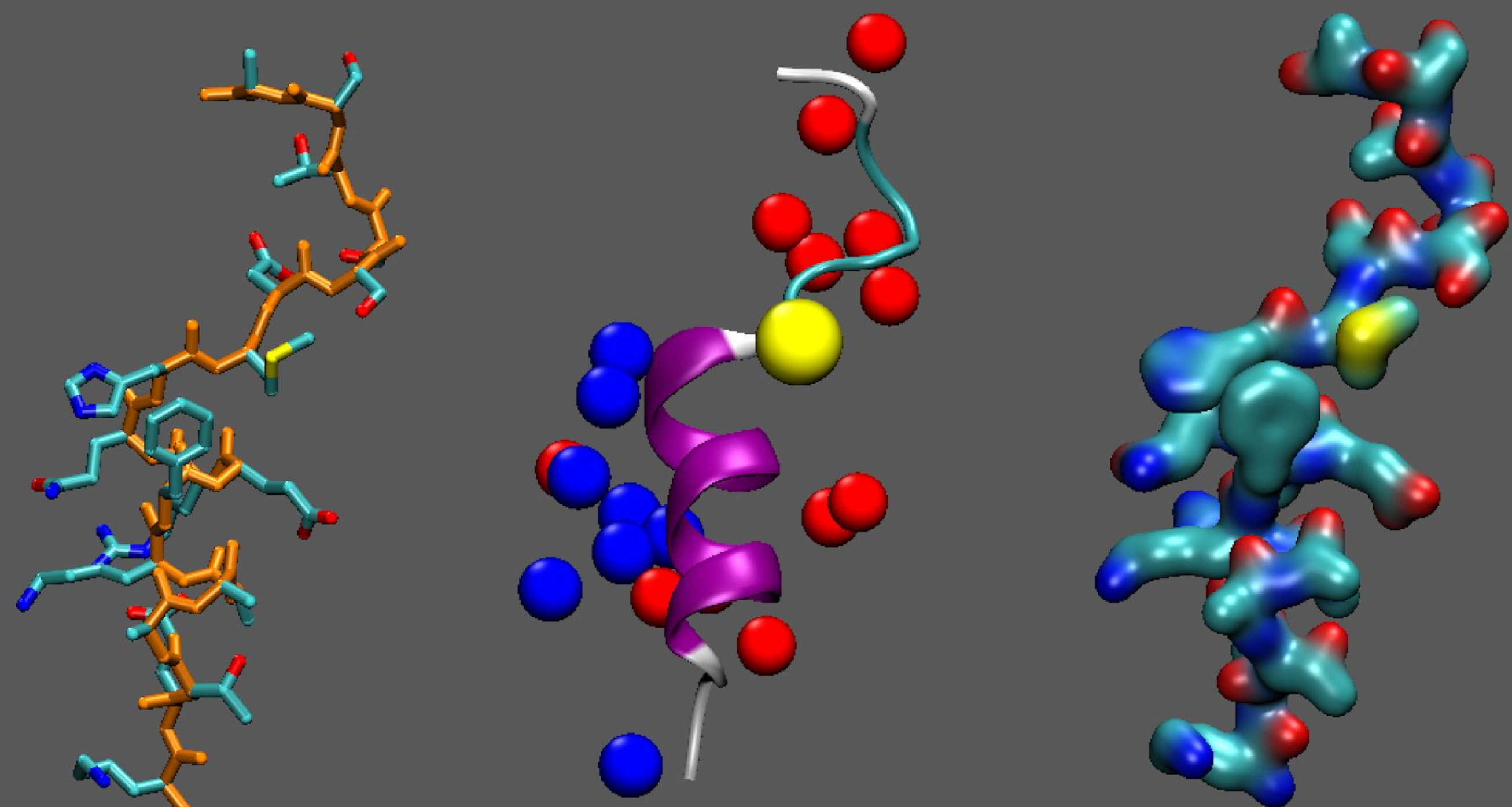
Macro definition:

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

- 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



A scrollable list box at the top of the dialog, currently empty.

Selected Atoms

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

Draw style | Selections | Trajectory | Periodic

Single word  
**predefined**  
selections

Singlewords

helix  
alpha\_helix  
helix\_3\_10  
pi\_helix  
sheet

and | or | not

Apply

Reset

Input buttons

Macro definition:

alpha\_helix

List of  
data fields,  
**keywords**

Keyword

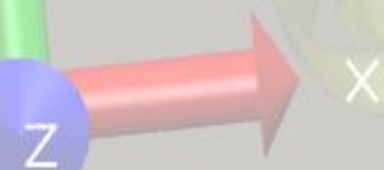
name  
type  
backbonetype  
residuetype  
index  
serial  
atomicnumber  
element  
residue

Value

NZ  
O  
OD1  
OD2  
OE1  
OE2  
OG  
OG1  
SD

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

**Current selection**





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 [Slider] zoom [ ] Loop [v] 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

Drawing Method VDW

Material Glass1

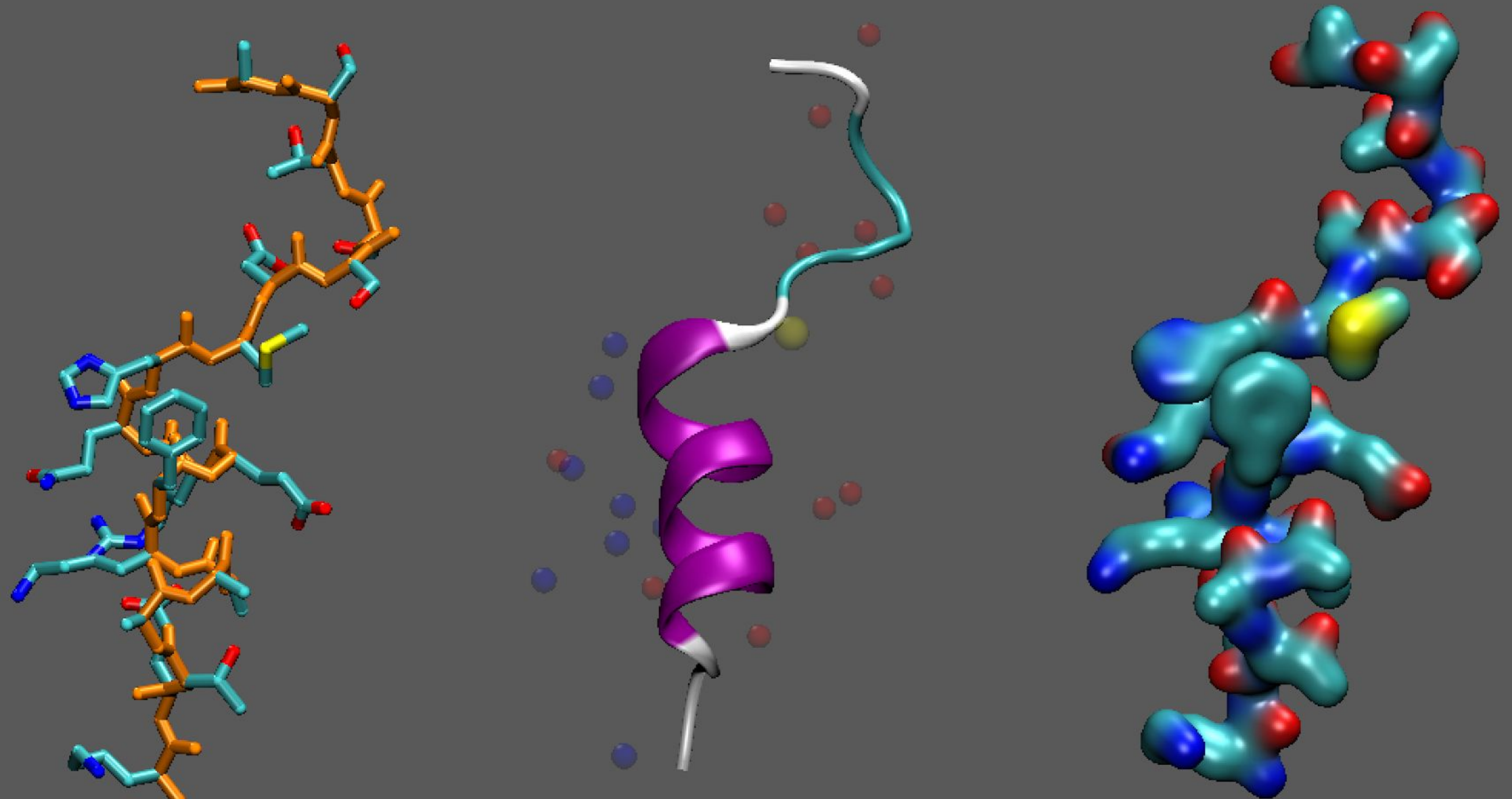
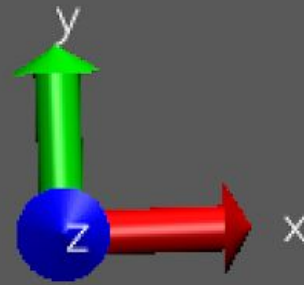
Default

Sphere Scale 0.4

Sphere Resolution 12

Apply Changes Automatically Apply

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



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

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

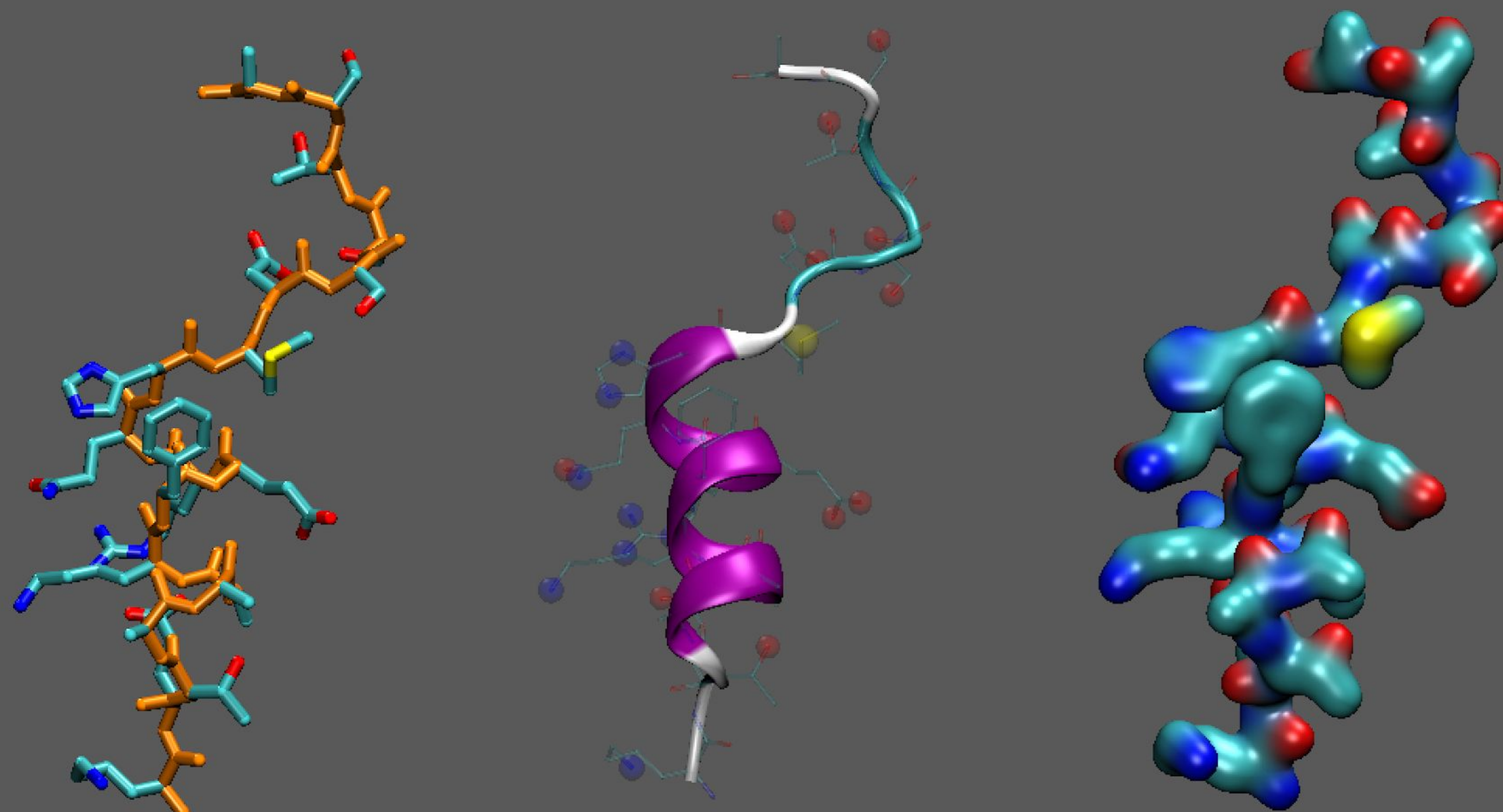
Sphere Resolution 12

Bond Radius 0.1

Bond Resolution 12

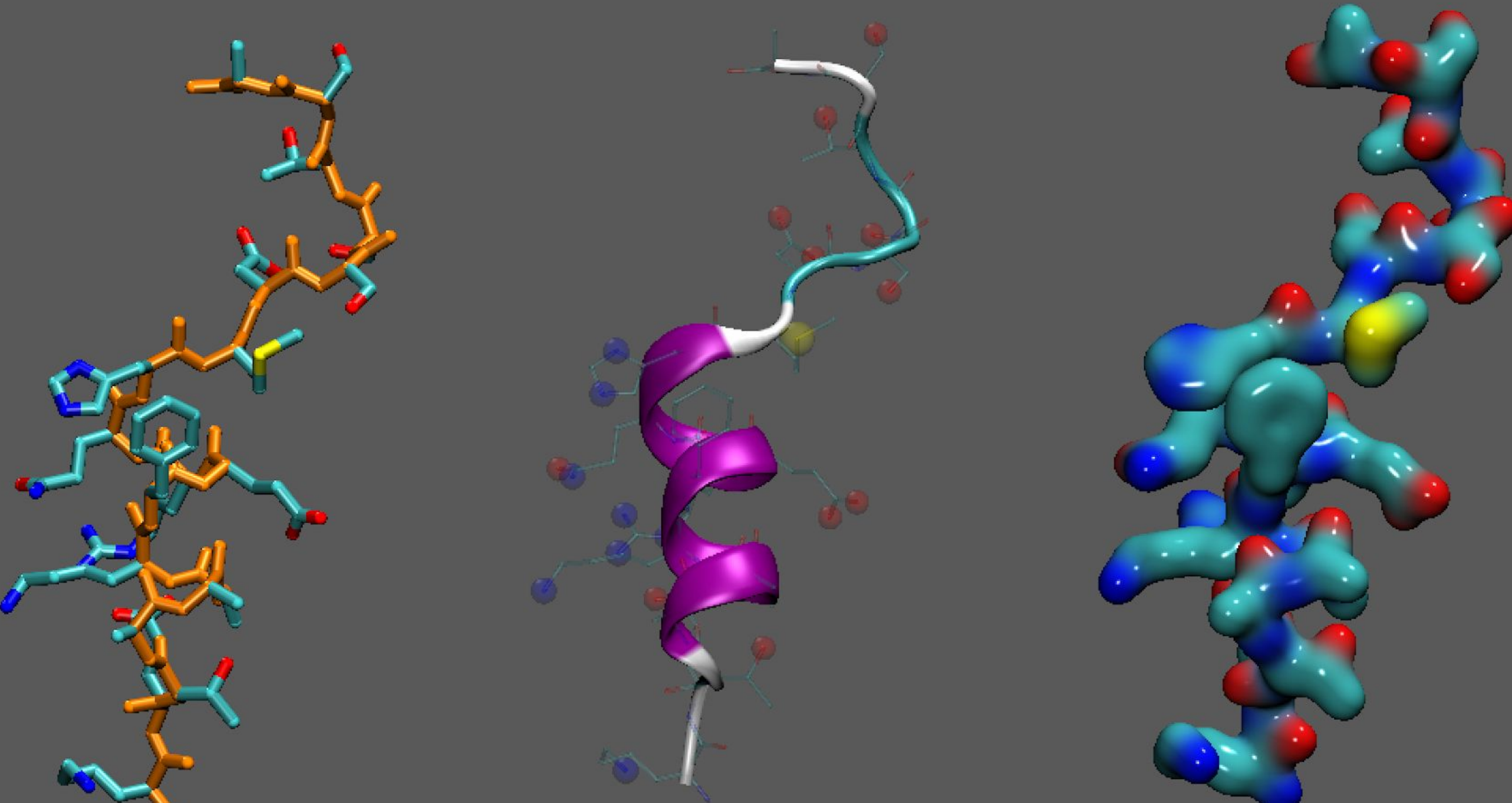
Apply Changes Automatically Apply

- 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



- 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

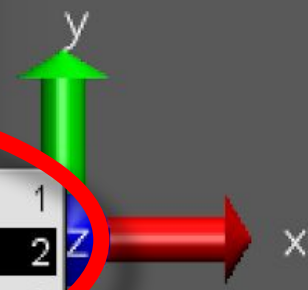
Selected Molecule  
2: speptide volume

Mouse Mode

- ☒ Rotate Mode R
- ☐ Translate Mode T
- ☐ Scale Mode S
- ☐ Center C
- ☐ Query Q
- ☒ Label L
- ☐ Move M
- ☐ Force F
- ☐ Move Light
- ☐ Add/Remove Bonds
- ☐ Pick P

Label Sub-menu:

- ☐ Atoms 1
- ☒ Bonds 2
- ☐ Angles 3
- ☐ Dihedrals 4



- 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.

Create Rep Delete Rep

Style	Color	Selection
QuickSurf	Name	all

Selected Atoms  
all

Draw style Selections Trajectory Periodic

Coloring Method  
Name

Drawing Method  
QuickSurf

Resolution 0.50

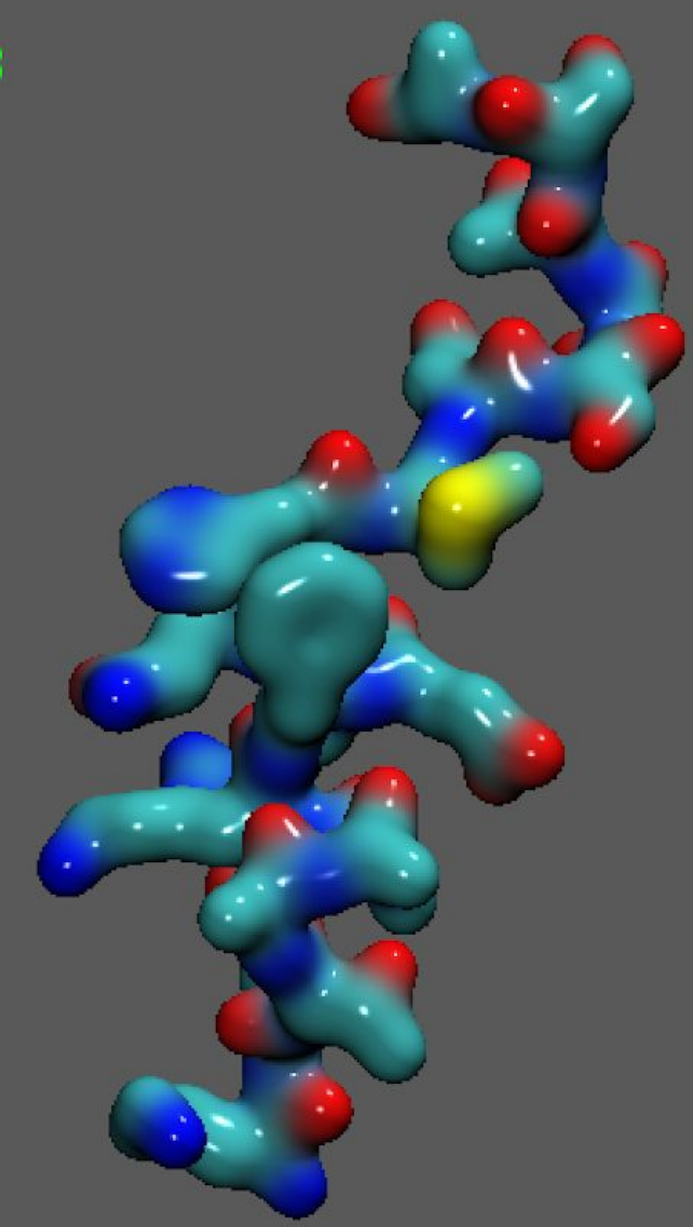
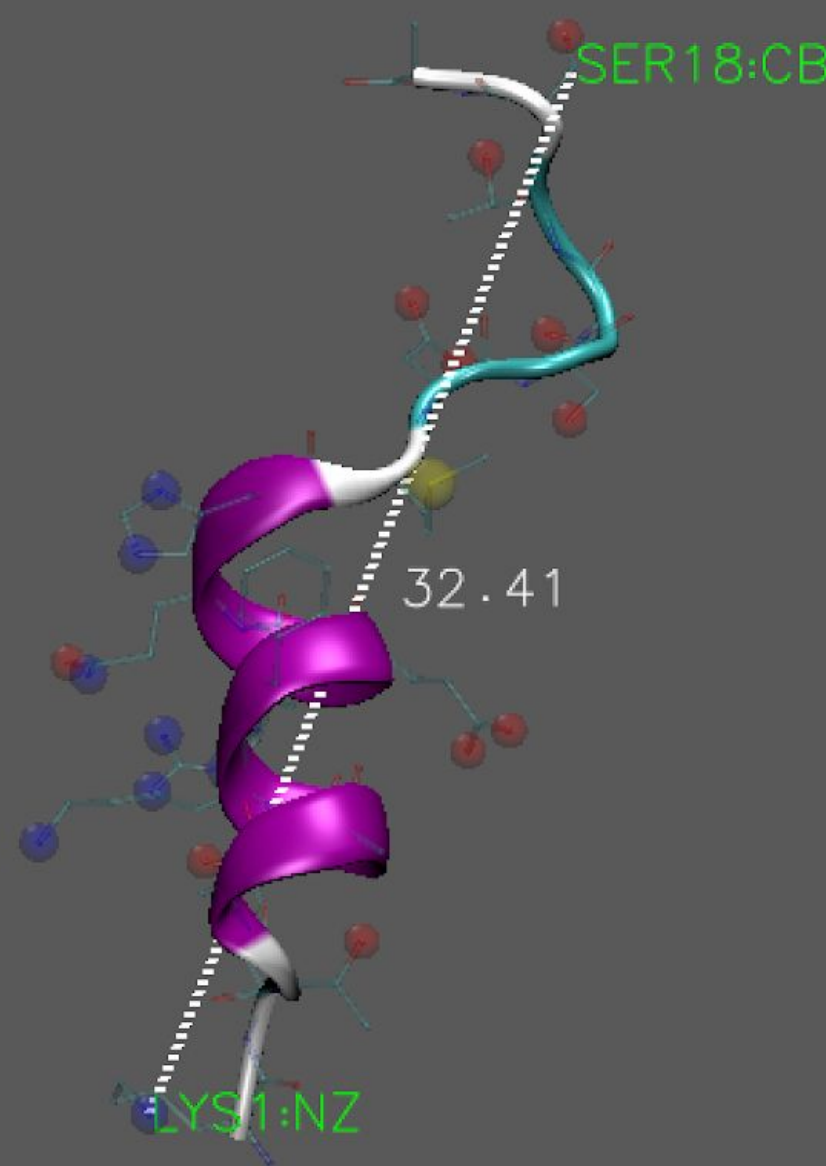
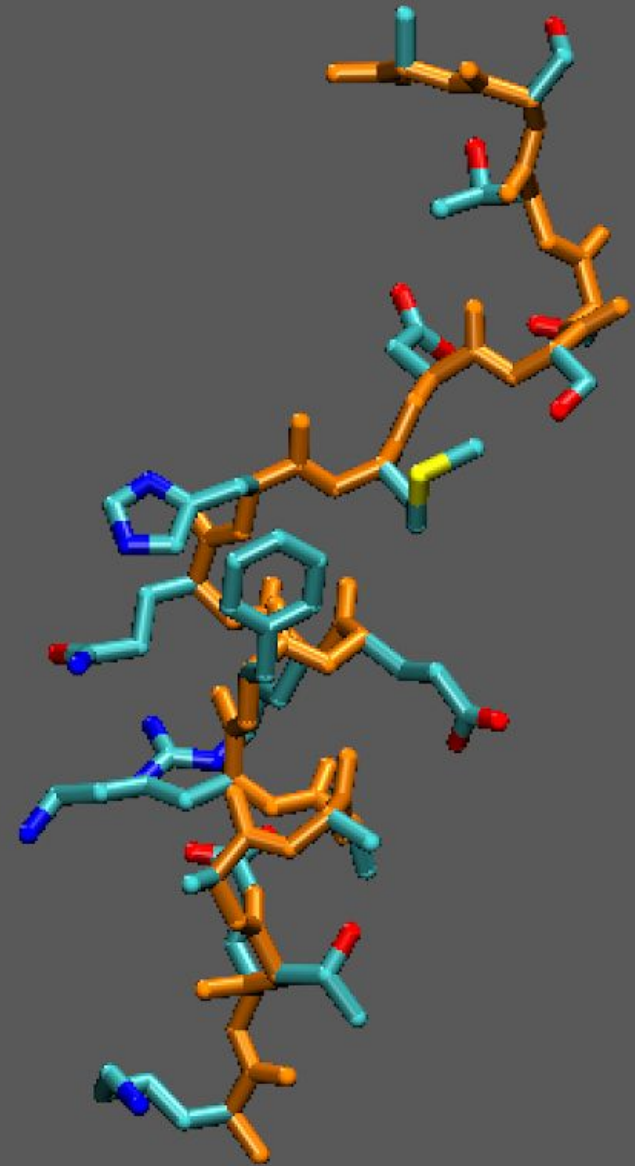
Radius Scale 0.5

Density Isovalue 0.5

Grid Spacing 0.2

Surface Quality Max


Apply Changes Automatically Apply

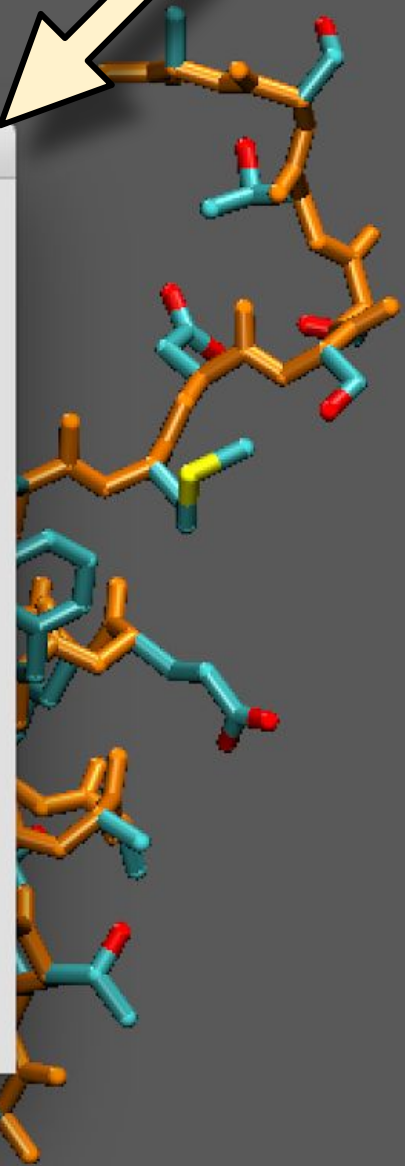


Working on an illustration



## Labels control window

- 



LYS1:NZ

# Working on an illustration



# Labels control

Floating dialog.  
Stays until closed.

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

Density Isovalue 0.5

Grid Spacing 0.2

Labels

Bonds

Show Hide Delete

LYS1:NZ SER18:CB

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: 32.414

Density Isovalue 0.5

Grid Spacing 0.2

- Delete atomic labels;
- Keep the bond label.



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 [Timeline bar] 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

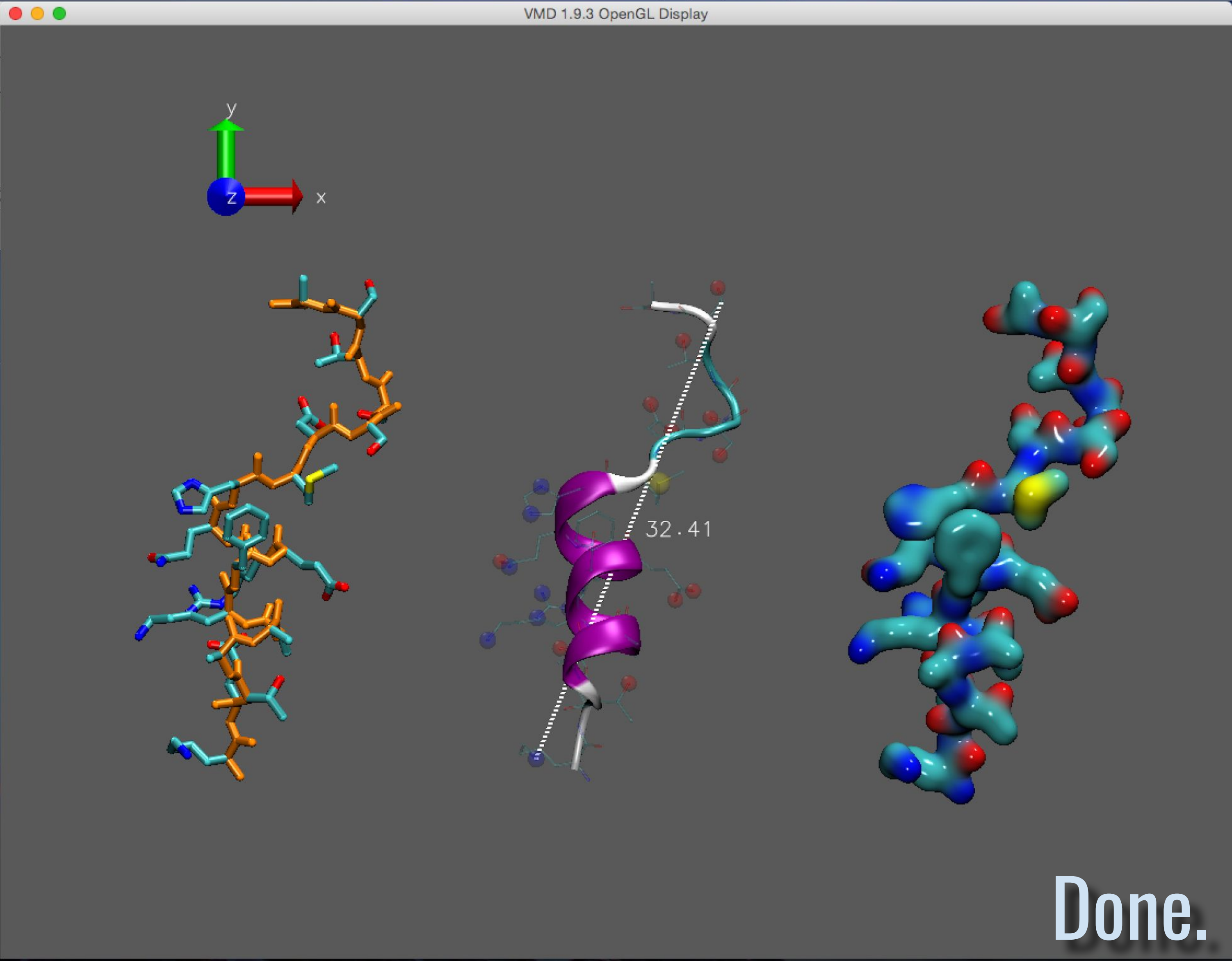
Radius Scale: 0.5

Density Isovalue: 0.5

Grid Spacing: 0.2

Surface Quality: Max

Apply Changes Automatically Apply



Done.

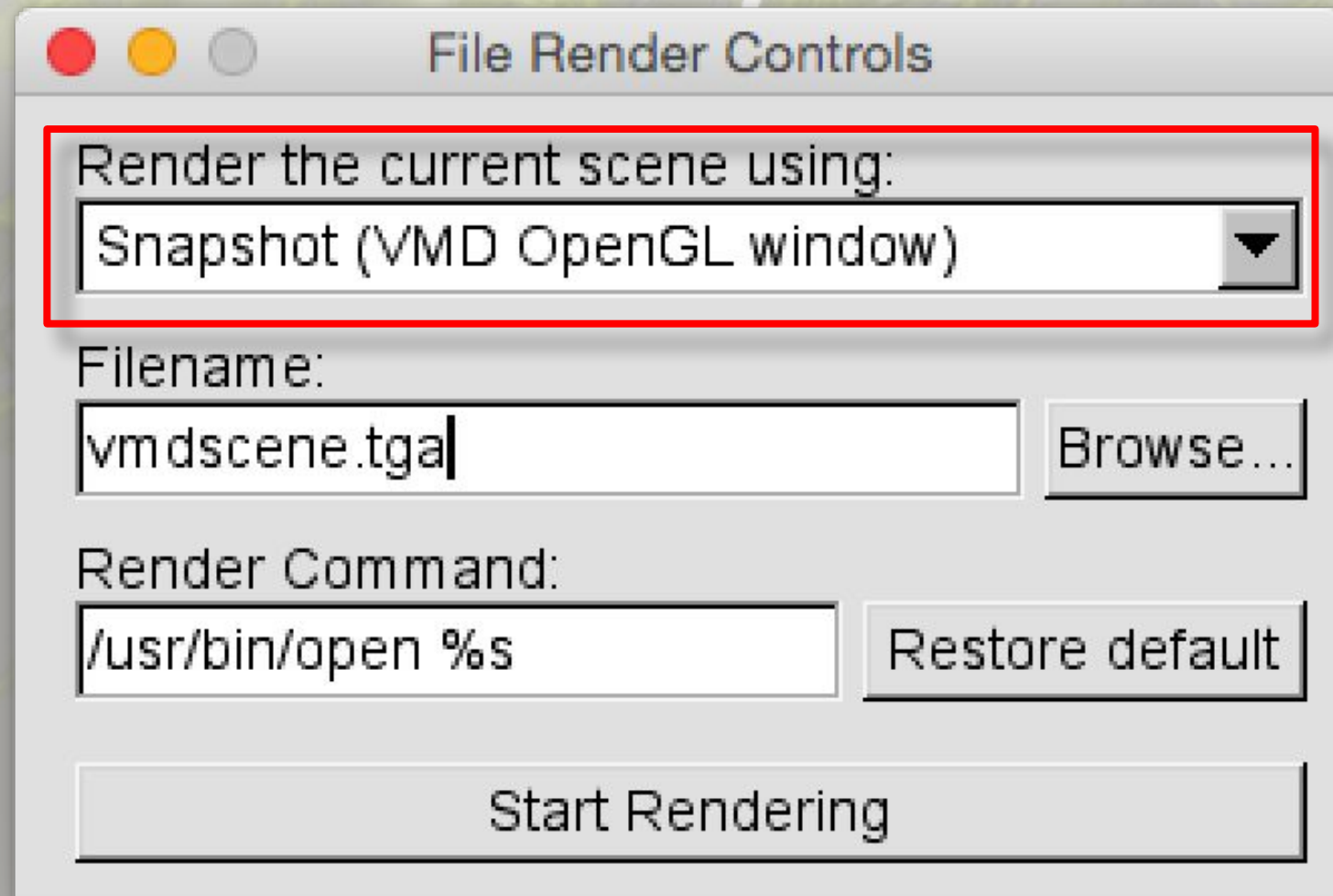


- 
- A 3D visualization of the electron density map of the 12S rRNA structure. The map is shown as a series of interconnected, elongated, and somewhat irregular shapes. The color scheme is primarily red and blue, with a prominent yellow region in the center. The red and blue areas represent different phases or components of the electron density, while the yellow region likely indicates a specific site of interest or a different phase. The overall structure is complex and multi-lobed, reflecting the intricate folding of the RNA molecule.

# Render it.



# Render dialog

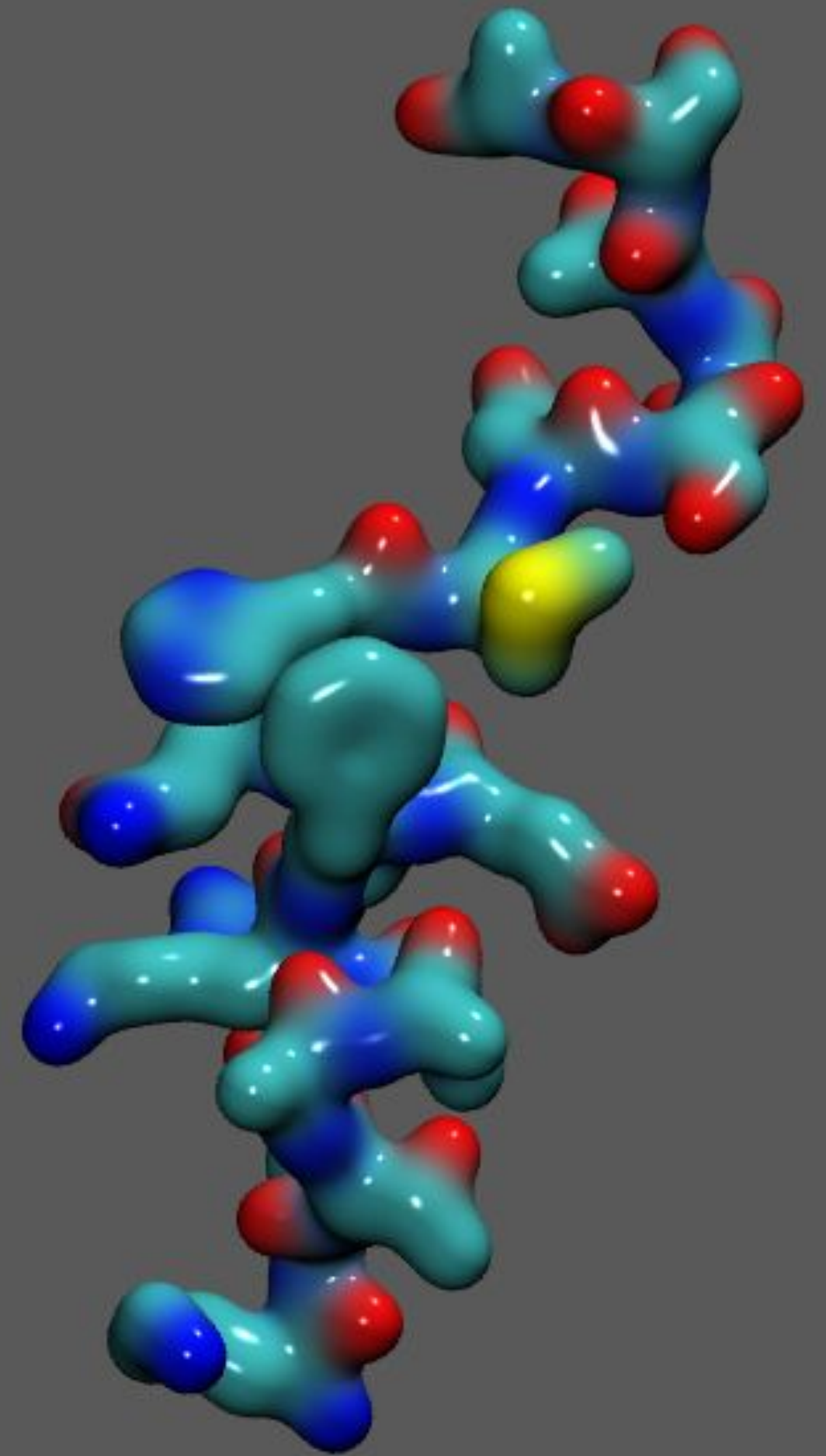
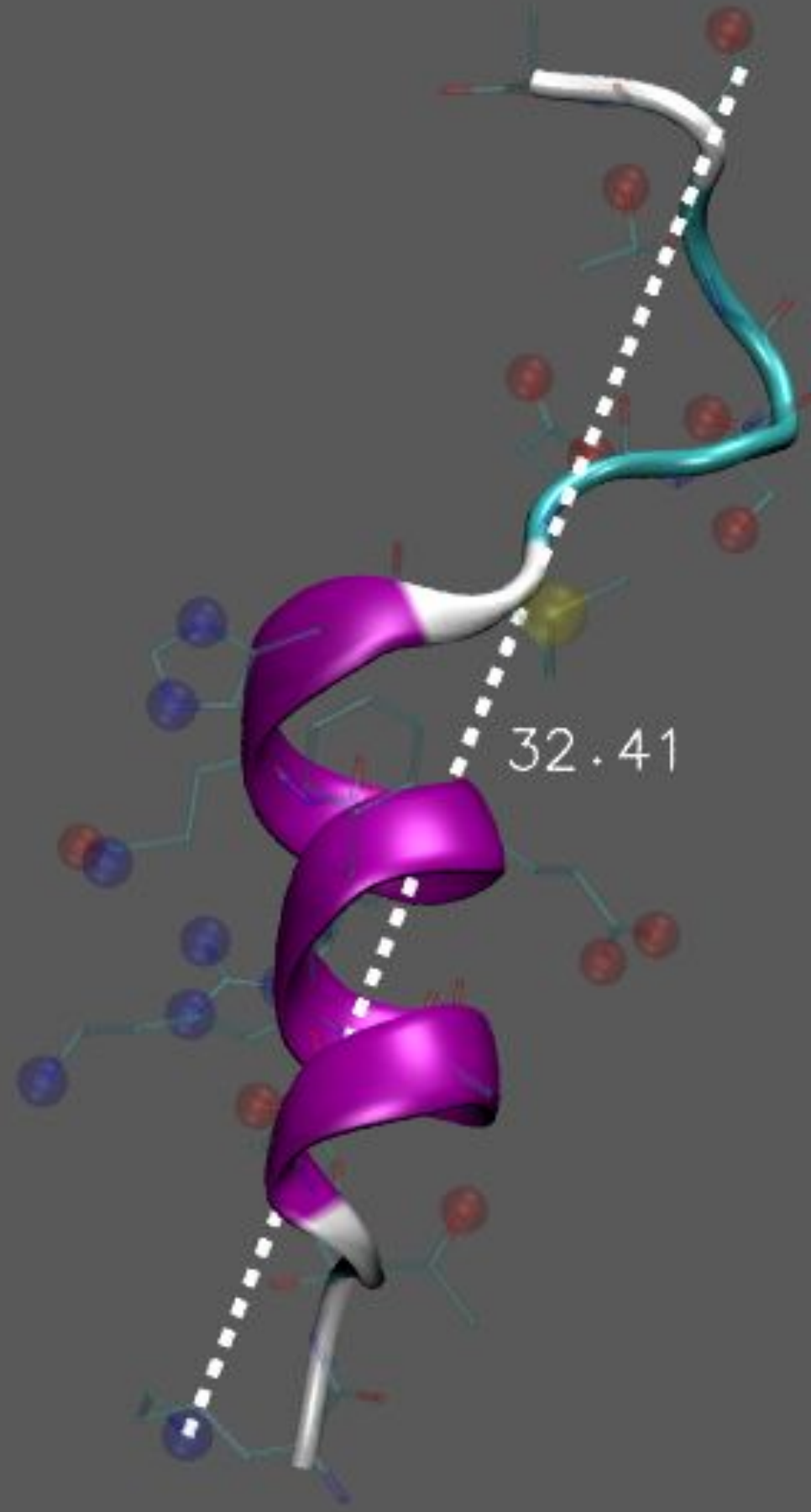
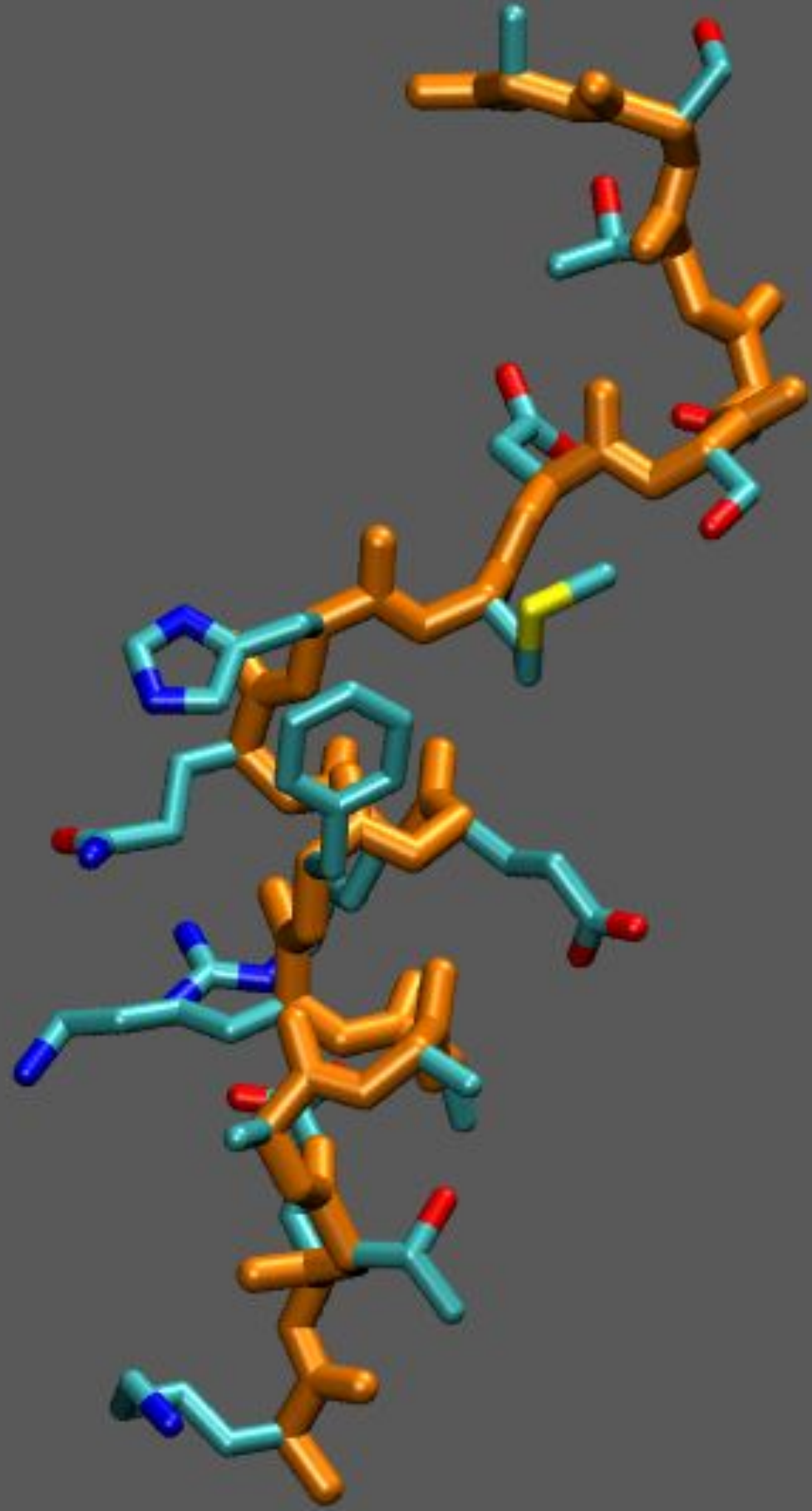


ART (VORT ray tracer)  
NVIDIA Gelato 2.1  
PostScript (vector graphics)  
Raster3D 2.7d  
Radiance 4.0  
Rayshade 4.0  
PIXAR RenderMan  
Snapshot (VMD OpenGL window)  
STL (triangle mesh only)  
Tachyon  
Tachyon (internal, in-memory rendering)  
POV-Ray 3.6  
VRML 1.0 (VRML94)  
VRML 2.0 (VRML97)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

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

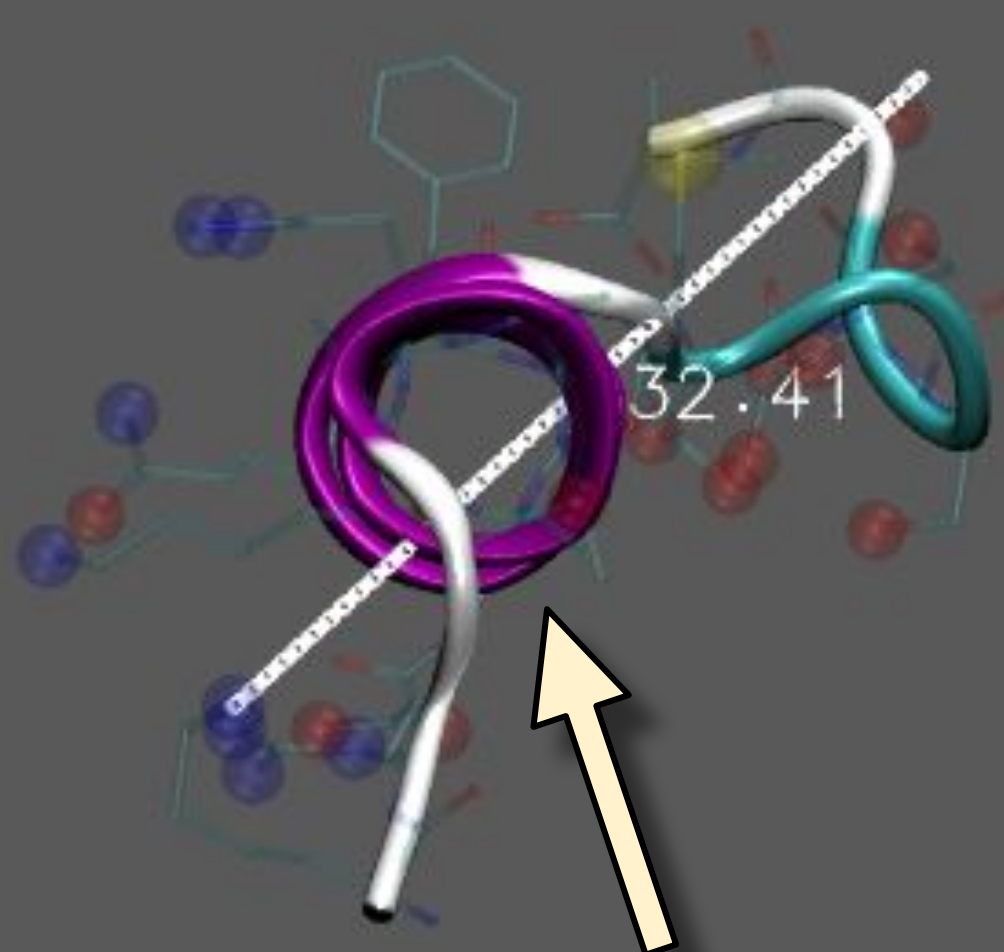
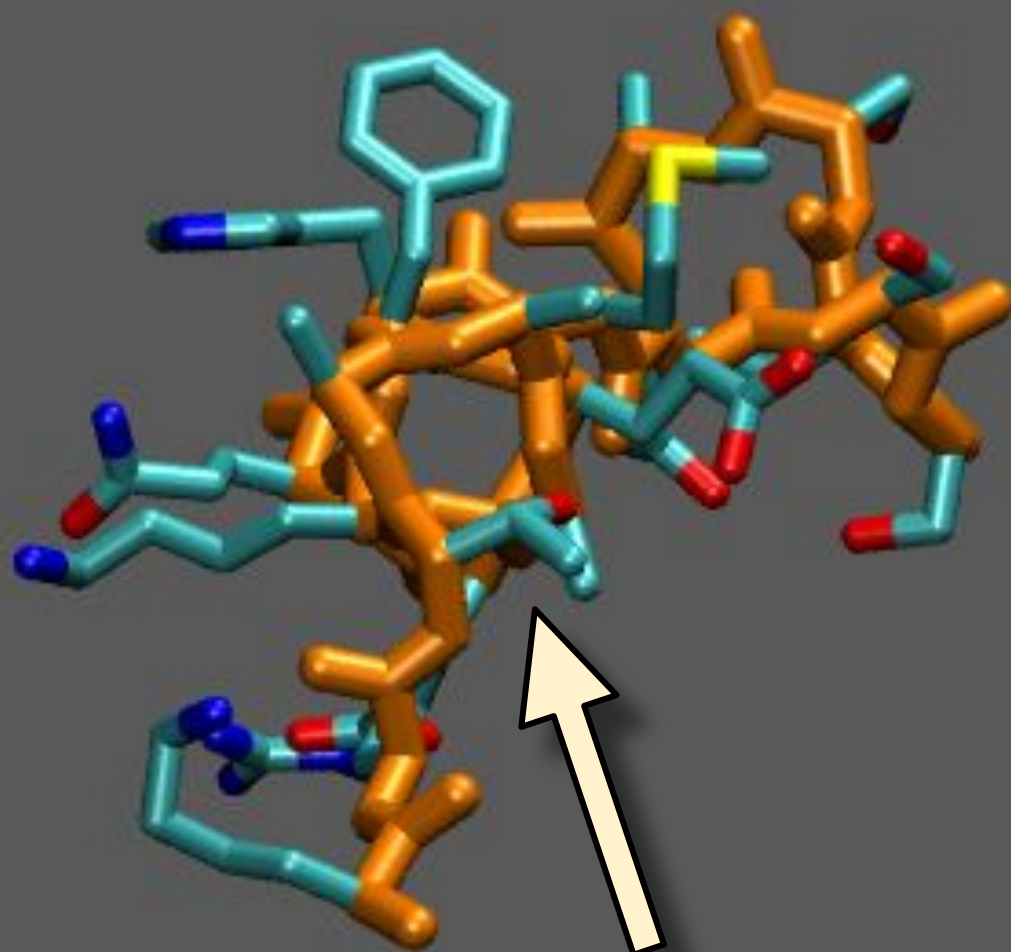


# Tachyon ray traced image

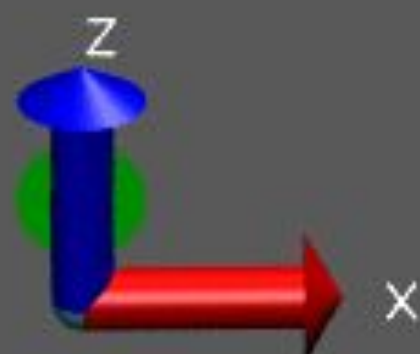
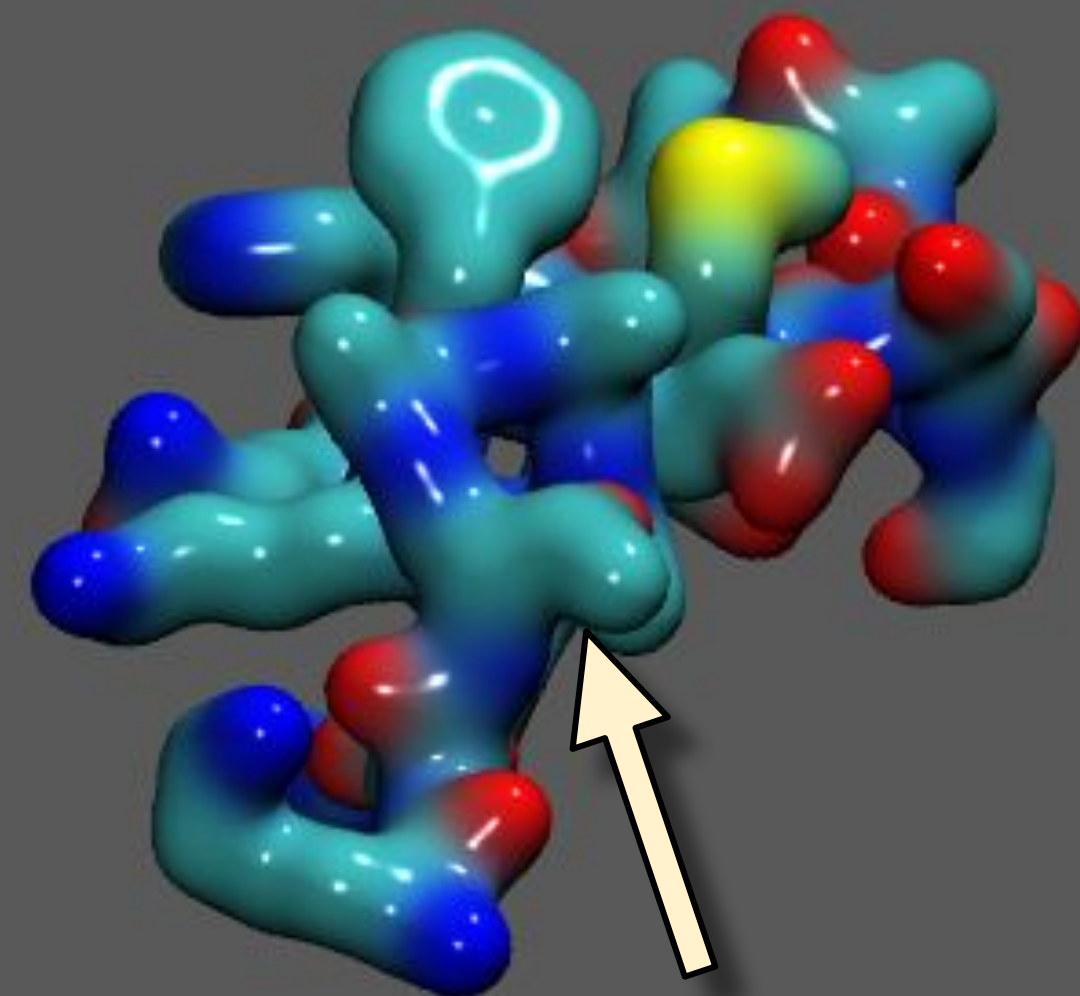




# Helix channel view



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](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!

