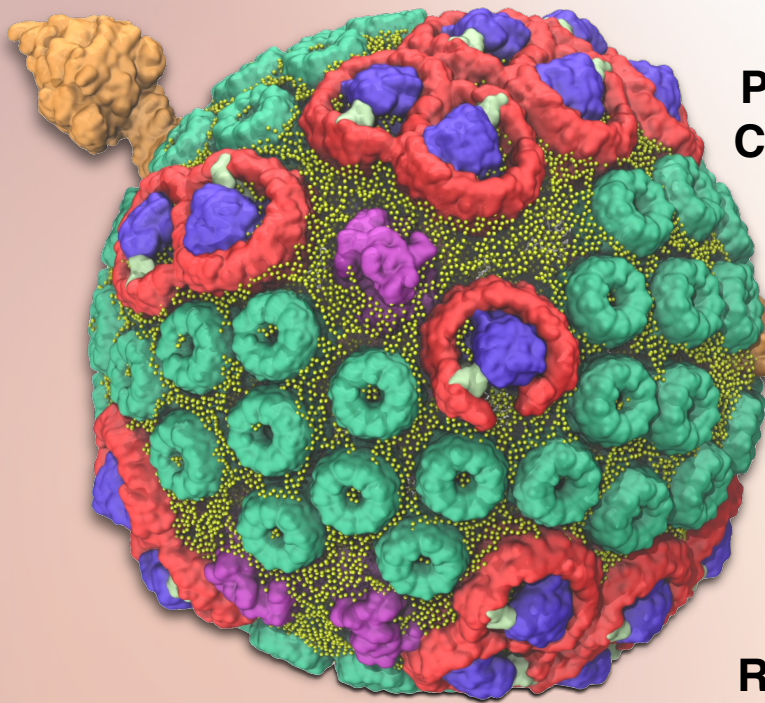


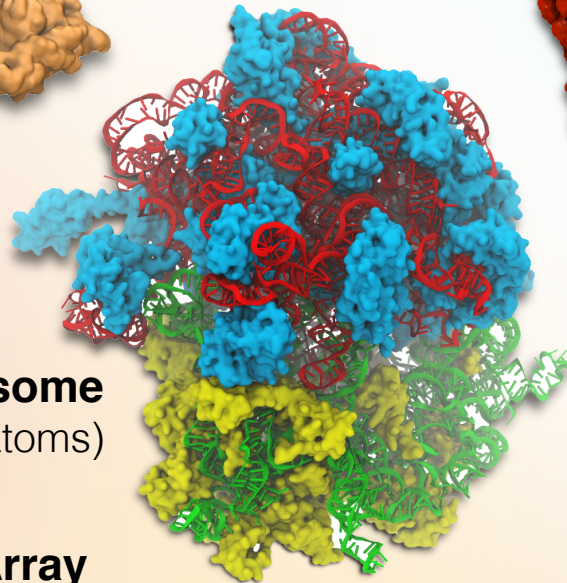
Tips and Tricks for Generating Images of Biomolecules in VMD

Jodi Ann Hadden

Workshop on Computational Biophysics

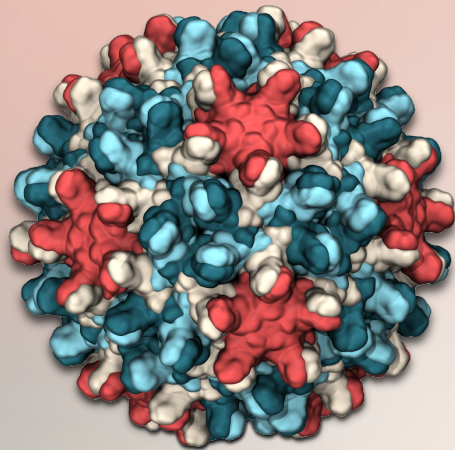
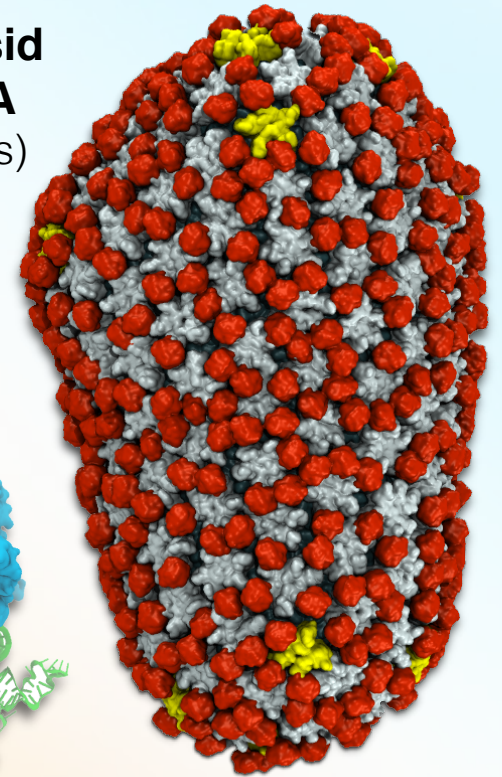


Photosynthetic Chromatophore
(100 M atoms)



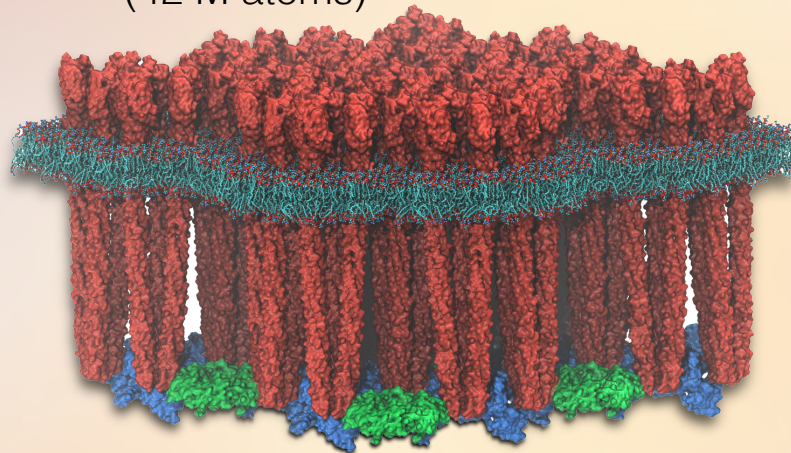
Ribosome
(4 M atoms)

HIV-1 Capsid with CypA
(64 M atoms)

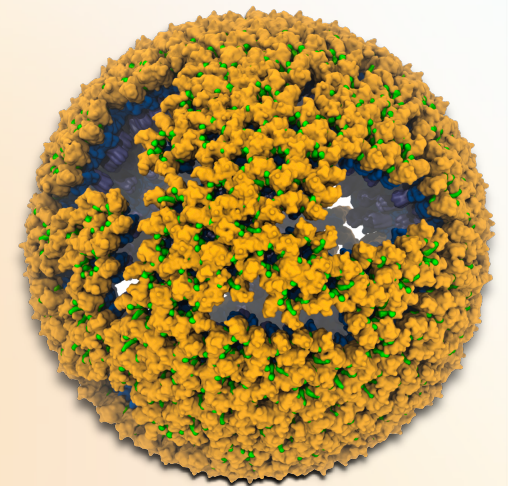


Hepatitis B Capsid
(6 M atoms)

Chemotactic Array
(42 M atoms)

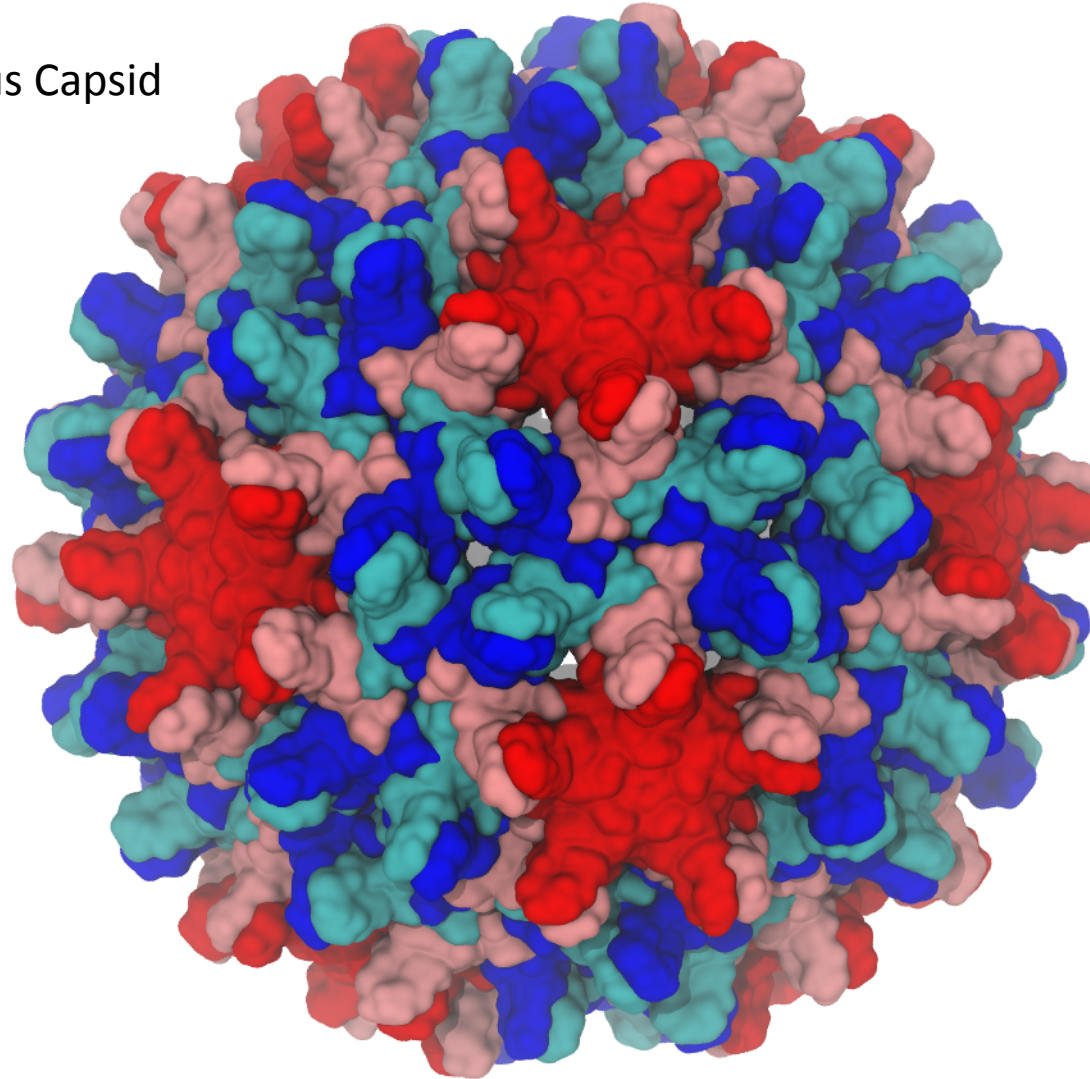


Immature Retroviral Capsid
(50 M atoms)



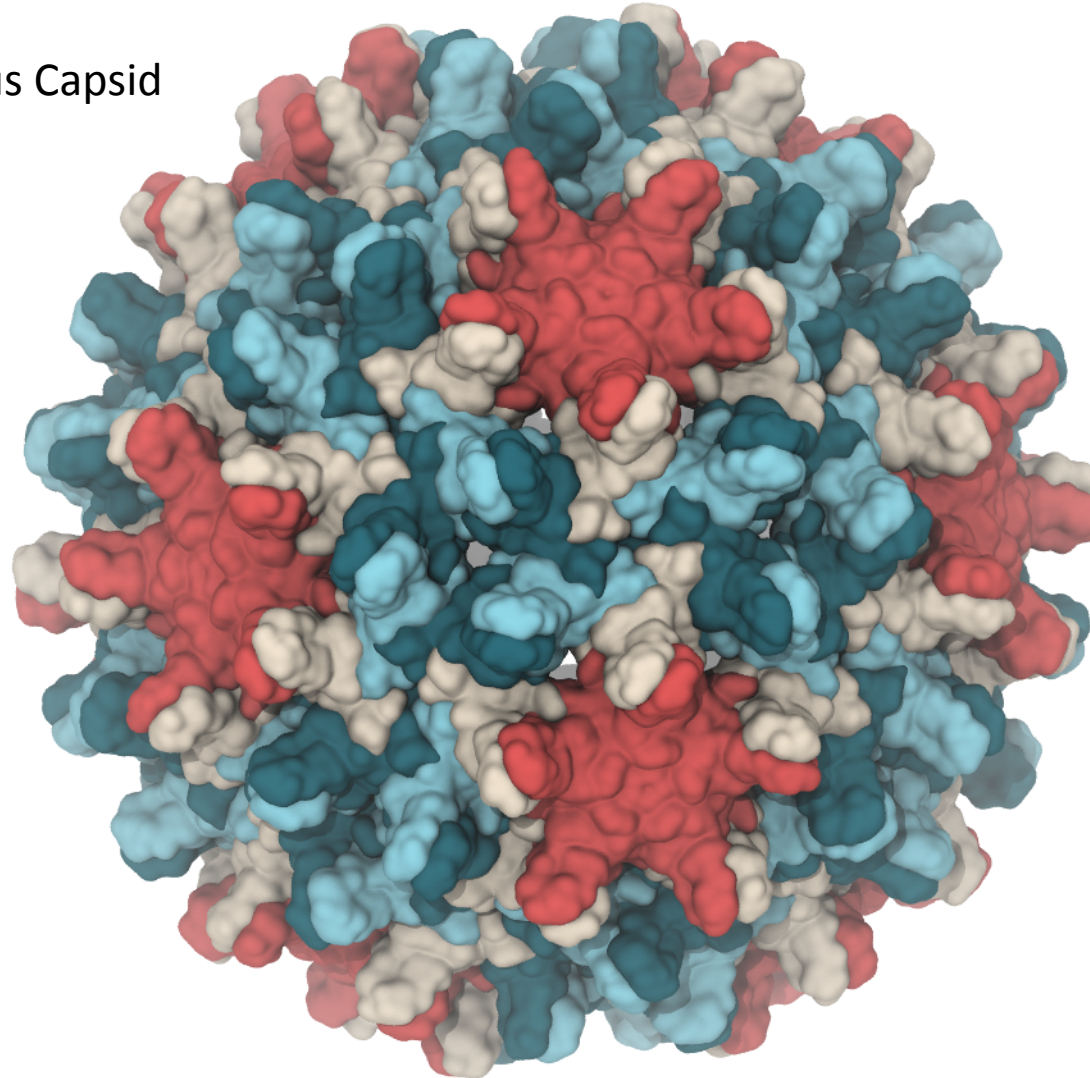
Don't use default VMD colors

Hepatitis B Virus Capsid

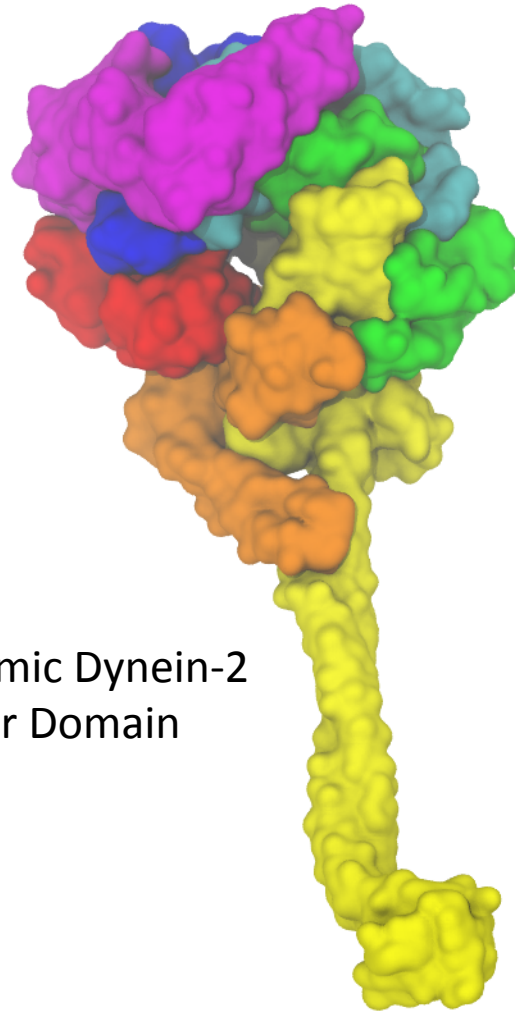


Don't use default VMD colors

Hepatitis B Virus Capsid

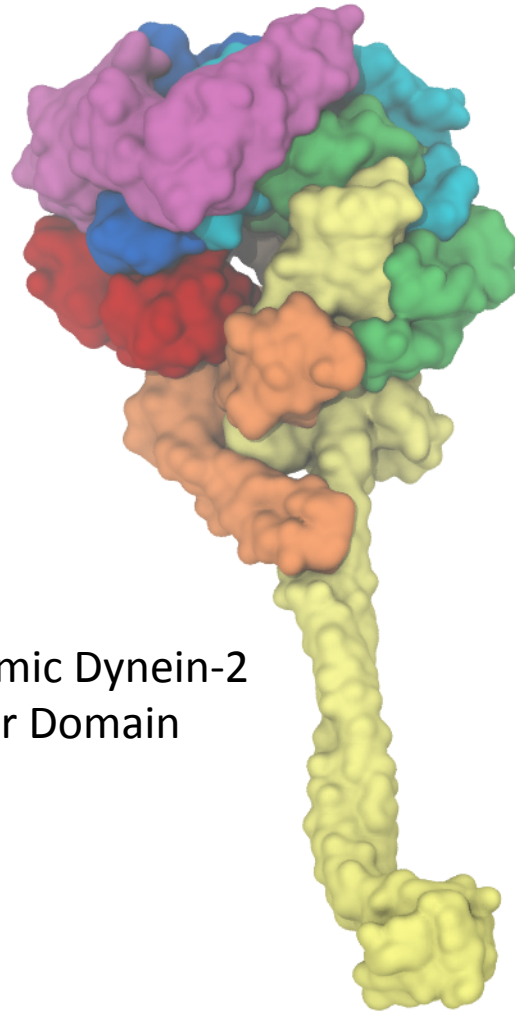


Don't use default VMD colors



Cytoplasmic Dynein-2
Motor Domain

Don't use default VMD colors



Cytoplasmic Dynein-2
Motor Domain

Color scheme/palette suggestions

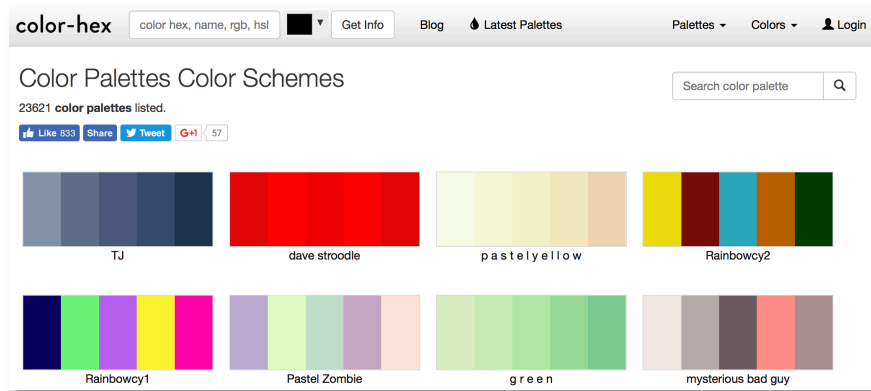
color-hex color hex, name, rgb, hsl Get Info Blog Latest Palettes Palettes Colors Login

Color Palettes Color Schemes

23621 color palettes listed.

Like 833 Share Tweet G+ 57

Search color palette

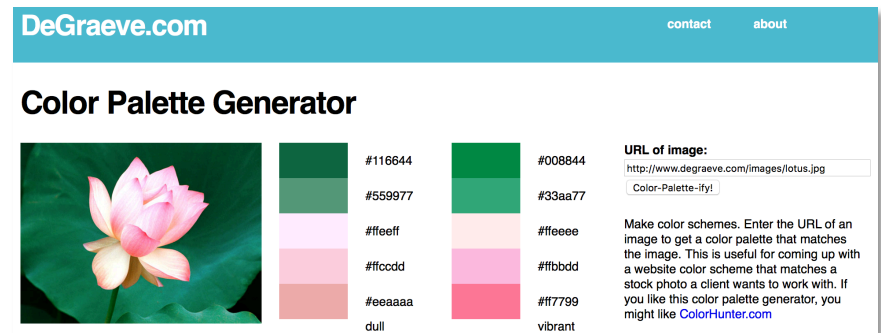


TJ dave stroodle pastelyellow Rainbowy2

Rainbowy1 Pastel Zombie green mysterious bad guy

DeGraeve.com contact about

Color Palette Generator



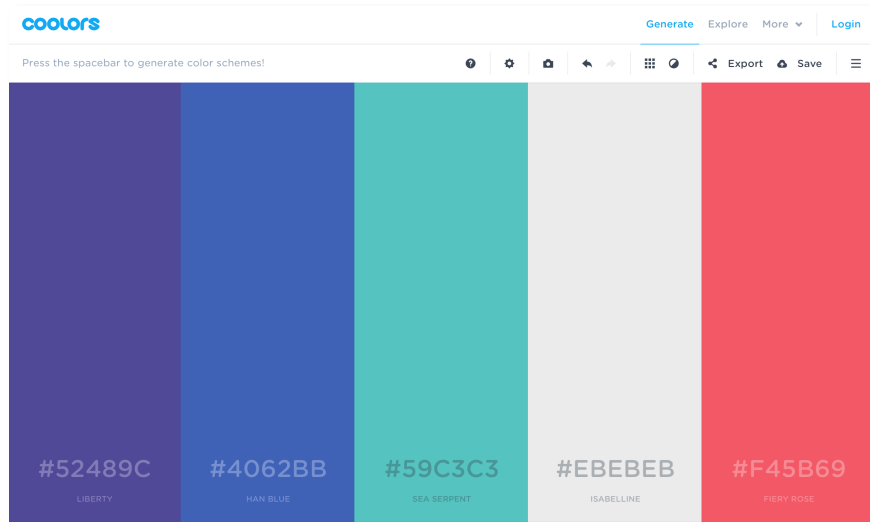
URL of image:

Make color schemes. Enter the URL of an image to get a color palette that matches the image. This is useful for coming up with a website color scheme that matches a stock photo a client wants to work with. If you like this color palette generator, you might like [ColorHunter.com](#)

#116644	#008844
#559977	#33aa77
#ffeeff	#f6eeee
#ffccdd	#ffb6dd
#eeaaaa dull	#ff7799 vibrant

coolors Generate Explore More Login

Press the spacebar to generate color schemes!



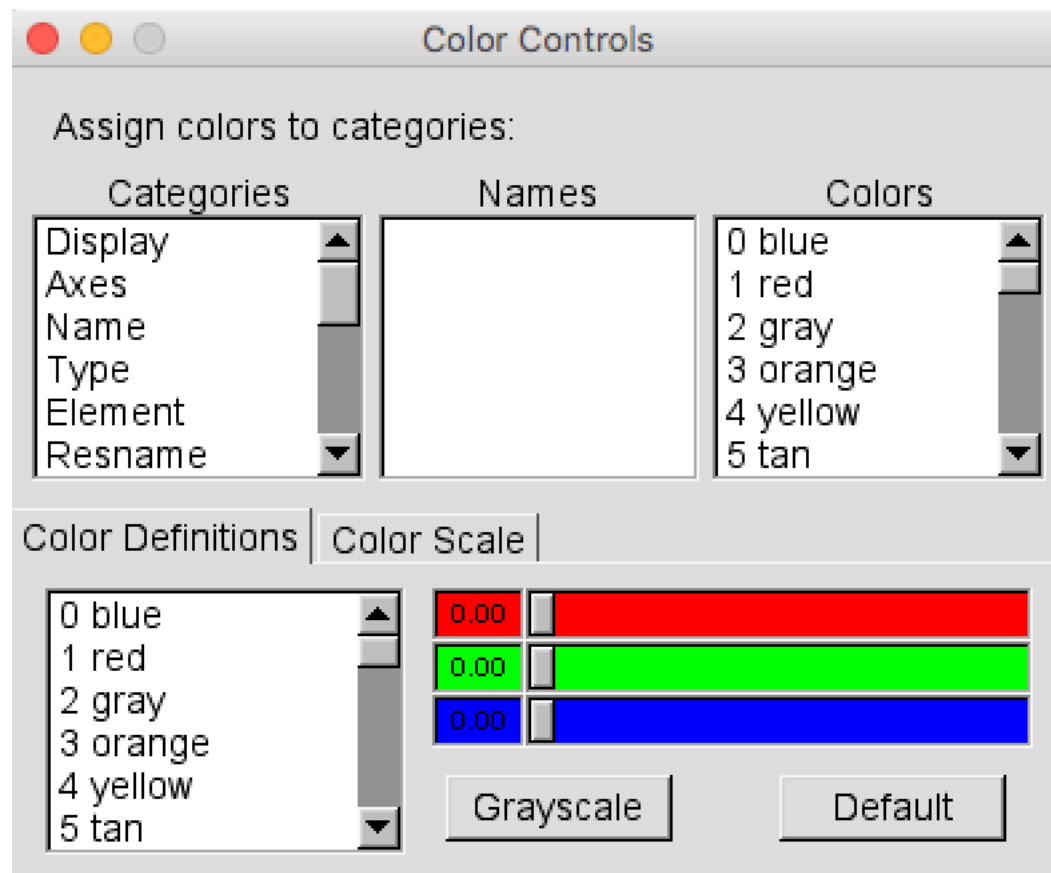
#52489C LIBERTY	#4062BB HAN BLUE	#59C3C3 SEA SERPENT	#EBEBEB ISABELLINE	#F45B69 FIERY ROSE
--------------------	---------------------	------------------------	-----------------------	-----------------------



Adobe
Capture CC

Applying color changes in VMD

```
color change rgb magenta [expr 207 / 255.] [expr 94 / 255.] [expr 181 / 255.]  
color change rgb blue [expr 0 / 255.] [expr 81 / 255.] [expr 203 / 255.]  
color change rgb cyan [expr 0 / 255.] [expr 204 / 255.] [expr 223 / 255.]
```

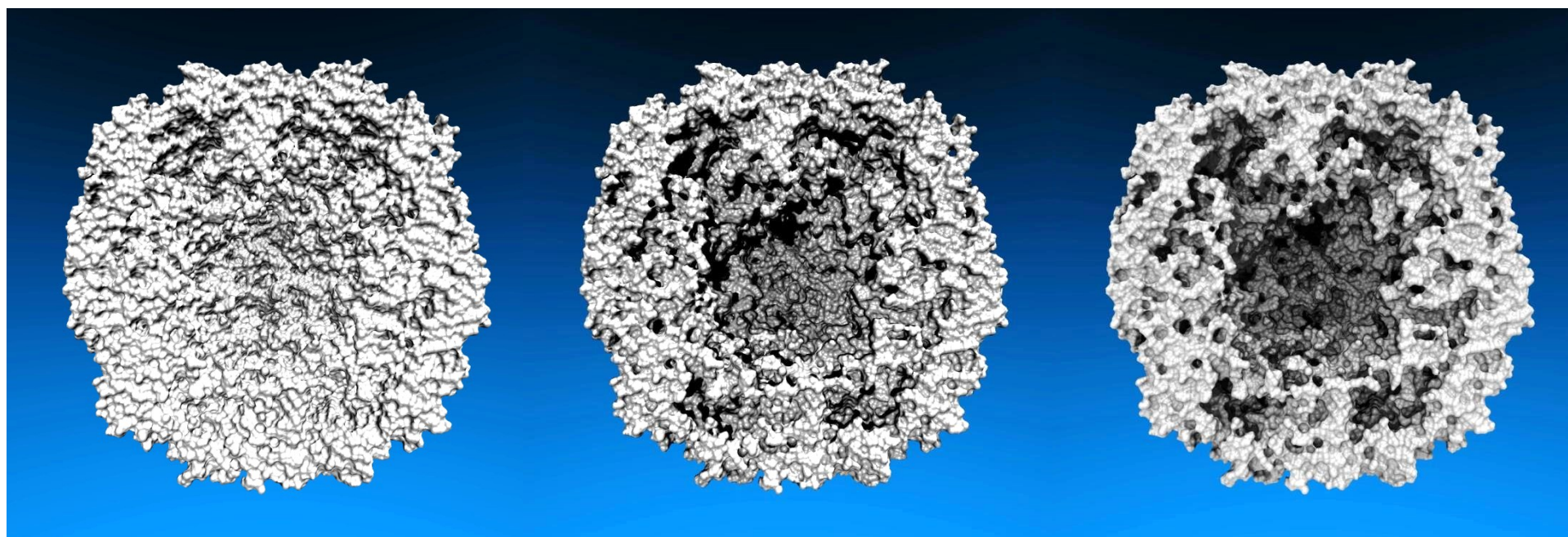


Lighting Comparison

Two lights, no shadows

Two lights, hard shadows, 1 shadow ray per light

Ambient occlusion + two lights, 144 AO rays/hit



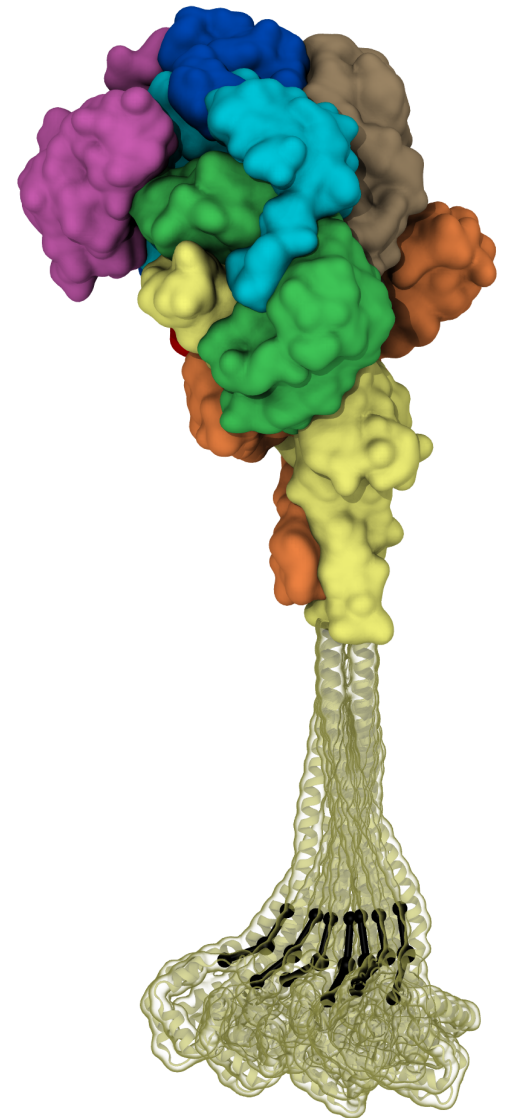
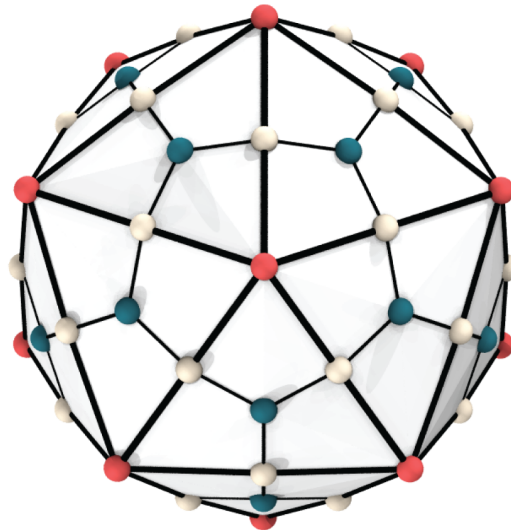
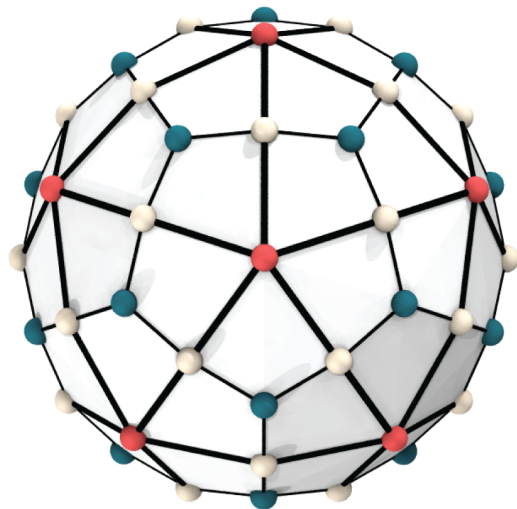
Shapes and Abstractions

```
set pt_a [measure center [atomselect top "chain A"]]  
set pt_b [measure center [atomselect top "chain B"]]  
set pt_c [measure center [atomselect top "chain C"]]
```

```
draw sphere $pt_a radius 5 resolution 25
```

```
draw cylinder $pt_a $pt_b radius 5 resolution 25
```

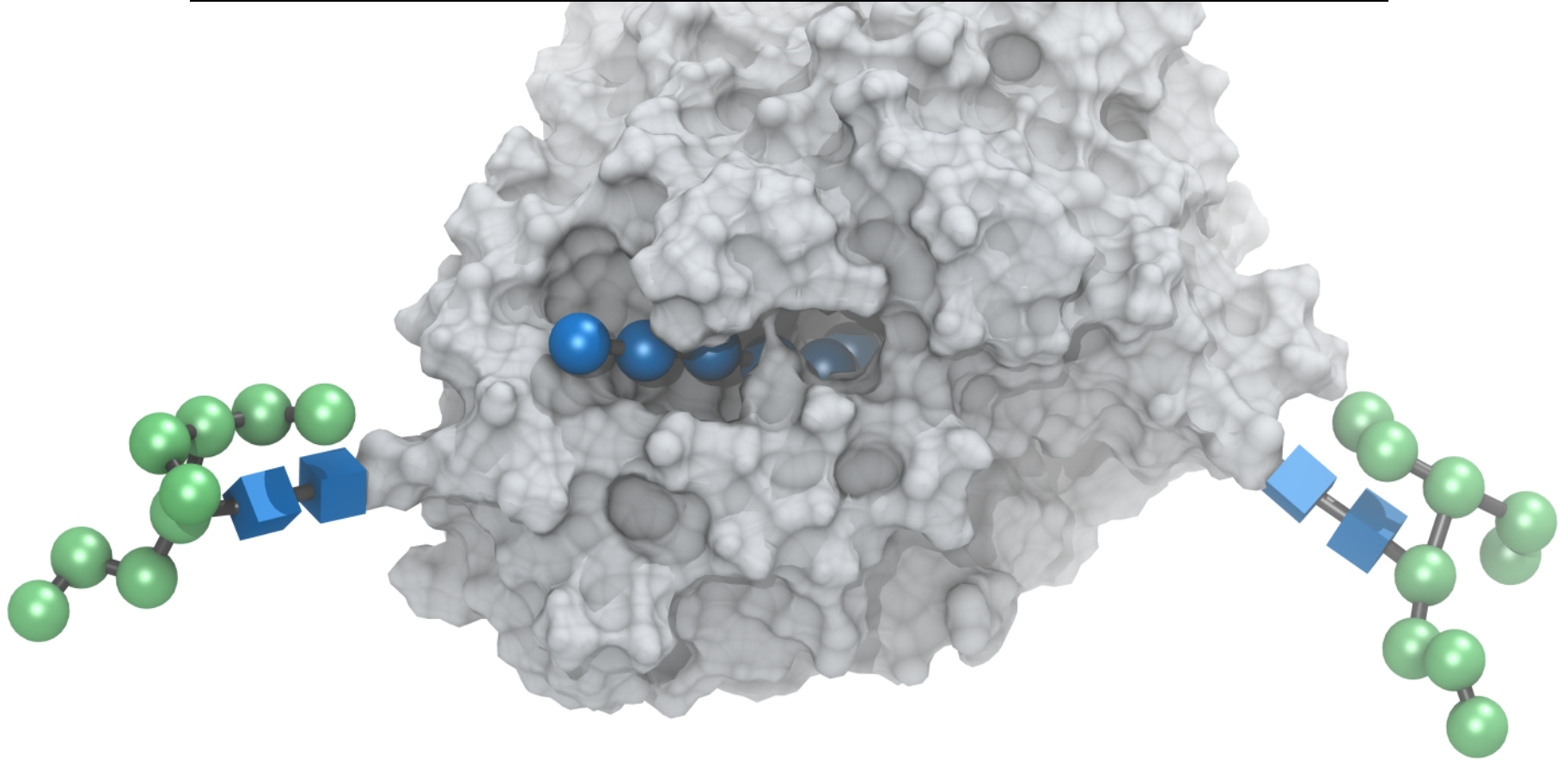
```
draw triangle $pt_a $pt_b $pt_c
```



Resolution and Rendering

- display resize x y
 - At least twice the size of your Photoshop canvas
- Render with Tachyon!
 - Materials look different when rendered
 - External Tachyon for transparency
 - trans_max_surfaces 1
- Save vmd state file to reload later
- Save tcl script to reproduce console commands

Live Demo: Visualizing Cel7A



Cellobiohydrolase complexed with cellonose
Glycosylated with Man9 *N*-glycans