eterna

Solve Puzzles. Invent Medicine.

Chimera Tutorial

How to use Chimera and ChimeraX to visualize 3D RNA structures

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Why should I care about 3D RNA structures?

- You don’t *have* to look at 3D structures to design RNA
- But sometimes things don’t make sense otherwise . . .

Example: “Outsider”

- Blog post by Nando (ElNando888)
- Saw this in a real-life structure:

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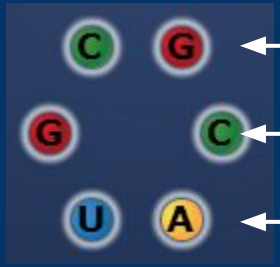


GC (paired) in a stack

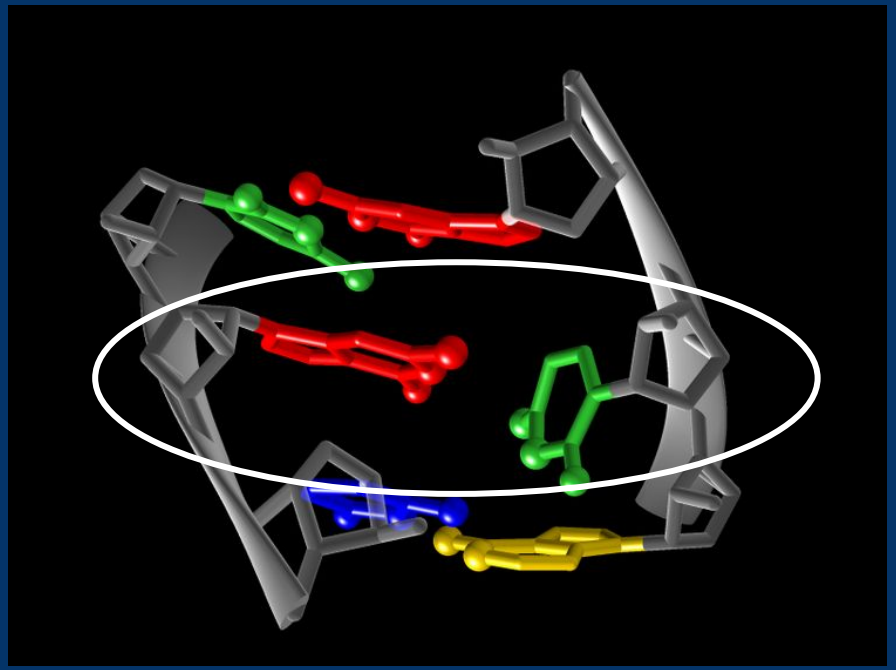
G and C in internal loop - not paired!

AU (paired) in a stack

- Our Eterna senses tell us this isn’t right! What’s going on?

A 3D view lets us directly observe base interactions.

- Here, the middle G and C are “tilted” in relation to each other



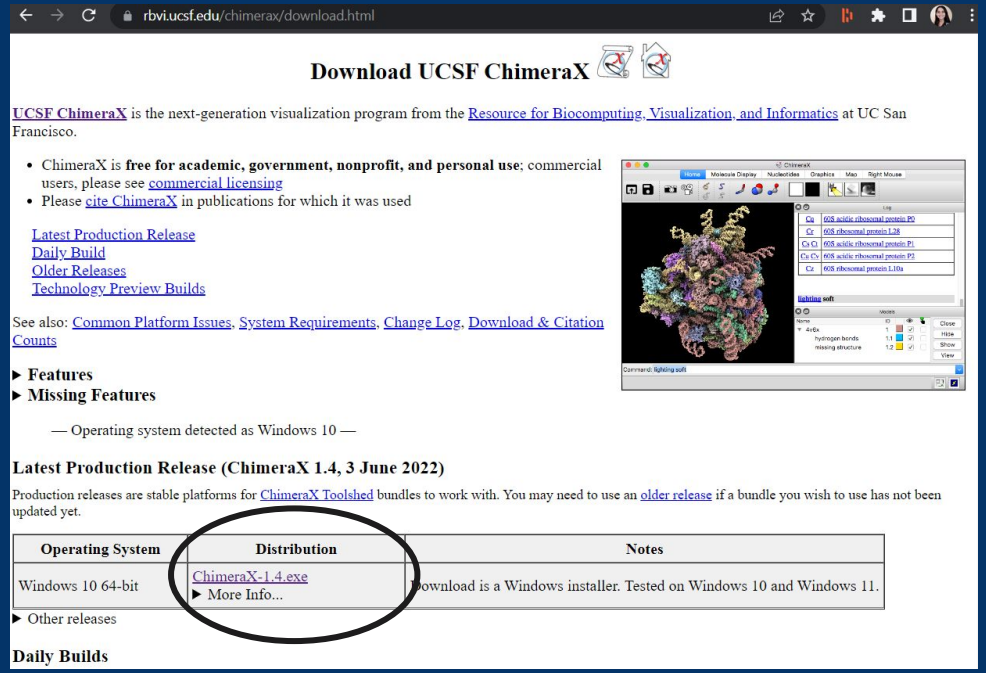
(PDB accession 3J2A,
residue 744 in chain N)

Seeing someone else's 3D structures is great; how do I look at 3D structures myself?

- Wide variety of 3D viewing programs available
- Today I'll be showing ChimeraX (which is very similar to Chimera)
  - Both from UCSF (University of California San Francisco)
  - Free!
- Will revisit Nando's example and see if we can replicate it ourselves

Installing ChimeraX (or Chimera)

- ChimeraX download page
  - I'll be using version 1.4 of ChimeraX
- Chimera download page
- Recommendation: use the production release for your operating system
  - If that doesn't work, try using a previously released version
- Note that this page also links to guides and tutorials
  - (Here, it's hidden under "Features")



rbvi.ucsf.edu/chimerax/download.html

Download UCSF ChimeraX

UCSF ChimeraX is the next-generation visualization program from the Resource for Biocomputing, Visualization, and Informatics at UC San Francisco.

- ChimeraX is **free for academic, government, nonprofit, and personal use**; commercial users, please see commercial licensing
- Please cite ChimeraX in publications for which it was used

Latest Production Release
Daily Build
Older Releases
Technology Preview Builds

See also: Common Platform Issues, System Requirements, Change Log, Download & Citation Counts

▶ **Features**
▶ **Missing Features**

— Operating system detected as Windows 10 —

Latest Production Release (ChimeraX 1.4, 3 June 2022)

Production releases are stable platforms for ChimeraX Toolshed bundles to work with. You may need to use an older release if a bundle you wish to use has not been updated yet.

Operating System	Distribution	Notes
Windows 10 64-bit	ChimeraX-1.4.exe ▶ More Info...	Download is a Windows installer. Tested on Windows 10 and Windows 11.

▶ Other releases

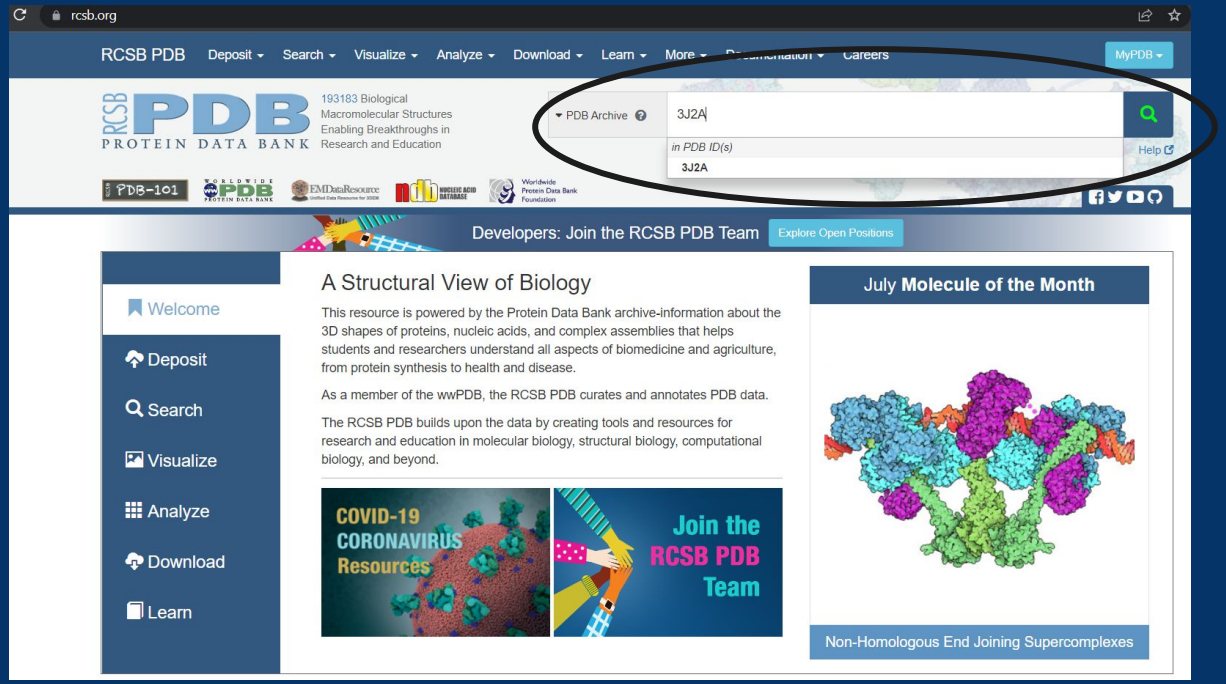
Daily Builds

Let’s start. First, I have to find a 3D file.

- Remember what Nando said: “PDB accession 3J2A, residue 744 in chain N”
- .pdb is a common 3D structure format; you might also see “mmCIF” (.cif) files
  - Both should load within ChimeraX

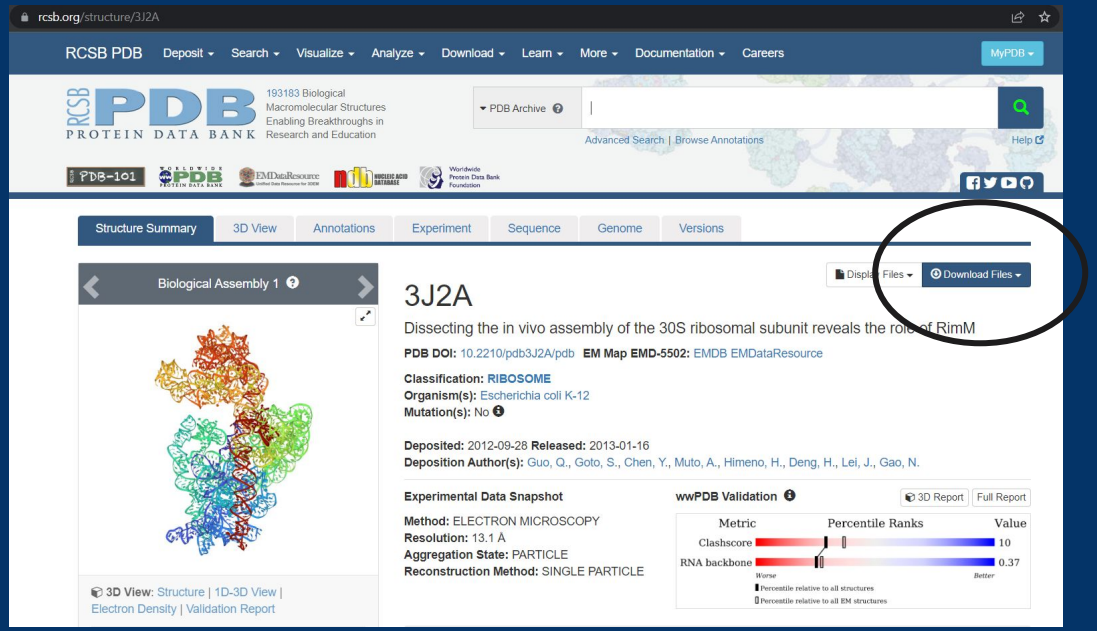
Finding the “3J2A” .pdb file

- RCSB PDB website
  - Type “3J2A” into search bar



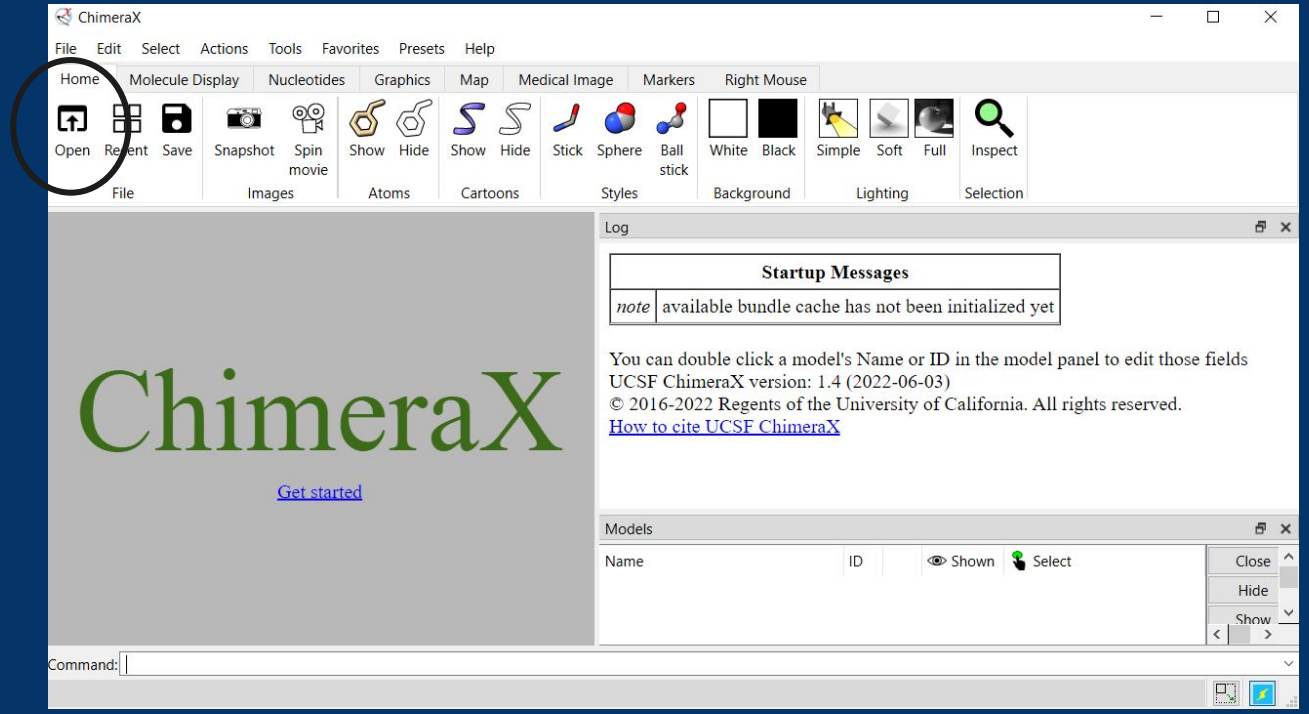
Finding the “3J2A” .pdb file

- This takes us to the 3J2A page
- Go to “Download Files” and choose “PDB Format”



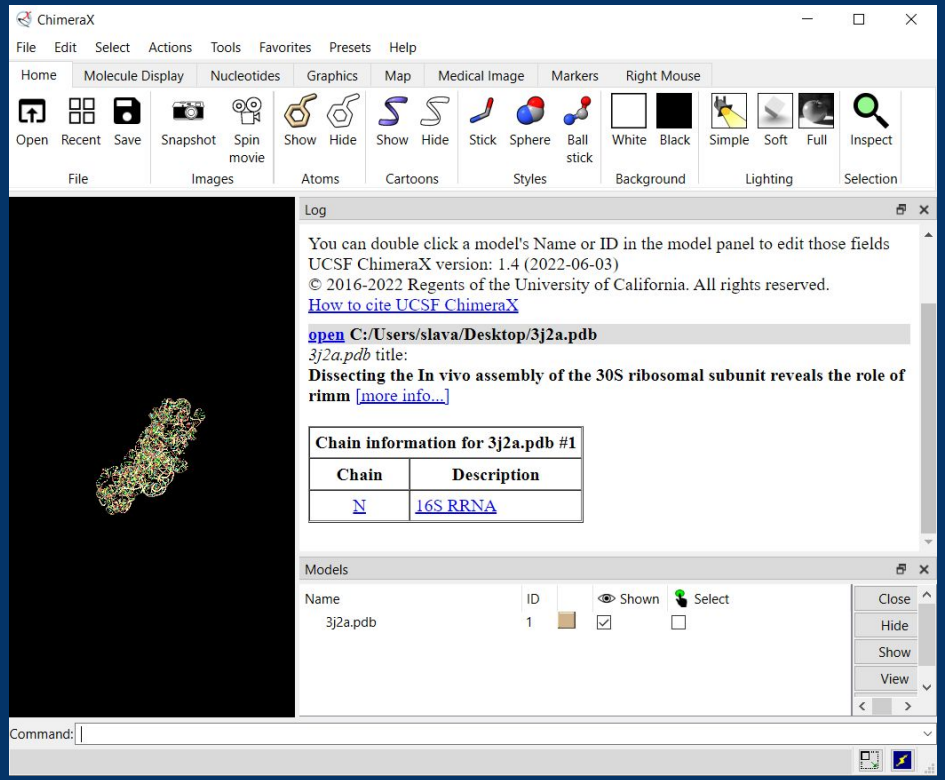
How do I load the 3D file into ChimeraX?

- Choose the “Open” option and choose our .pdb file



Great! . . . Now what?

- Let's adjust the view so we can actually see the RNA
- Controls (on Windows):
  - Click and drag to rotate
  - Mouse whee to zoom
  - Shift-click and drag to pan



Great! . . . Now what?

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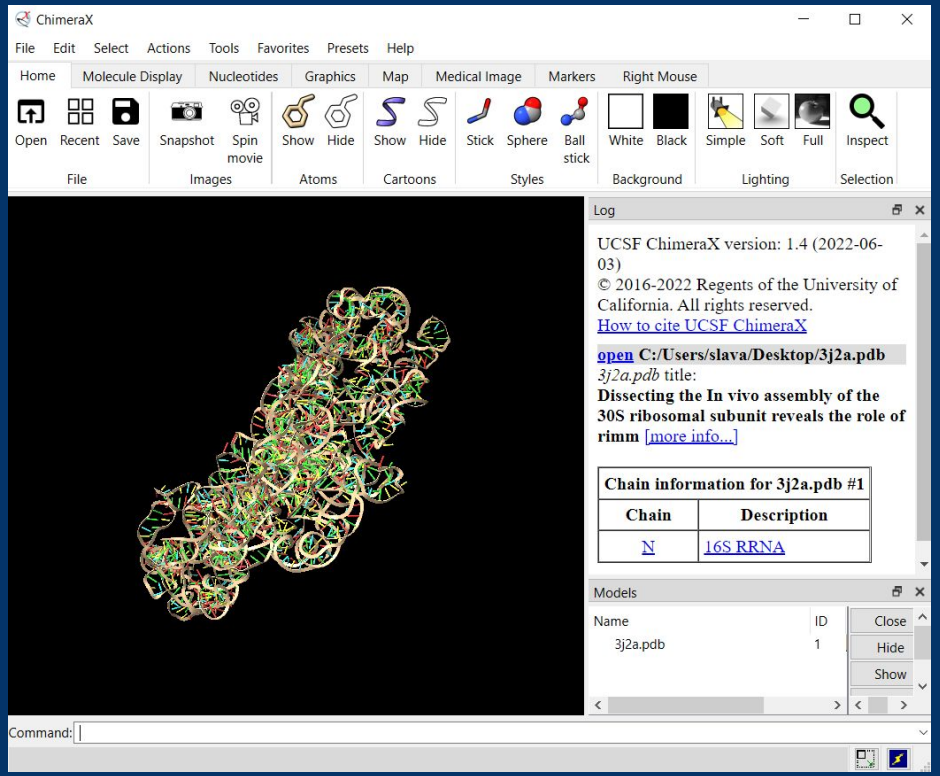
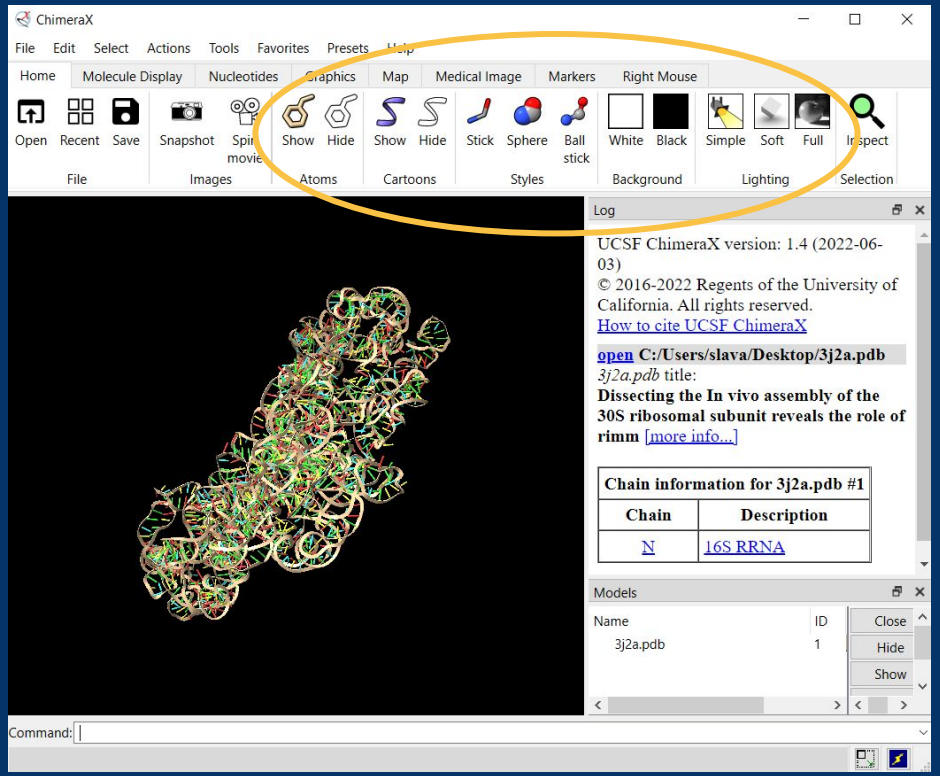
- Better!



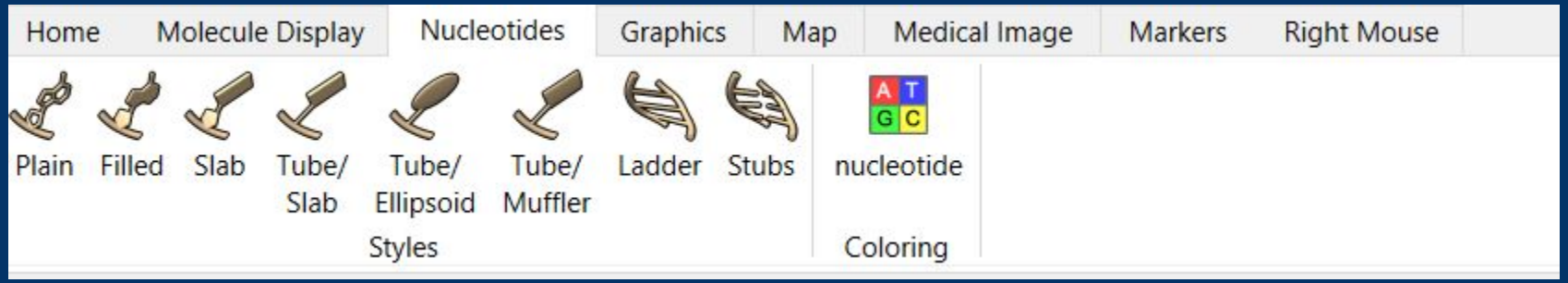
Using visual style options to better interpret 3D

- Basic visual options shown in top menu: Atoms, Cartoons, Styles, Background, and Lighting
  - Note: some (like styles) will only be noticeable if you show atoms
- More detailed visual options available in dropdown menus and tabs
- Experiment with what works for you!



Using visual style options to better interpret 3D

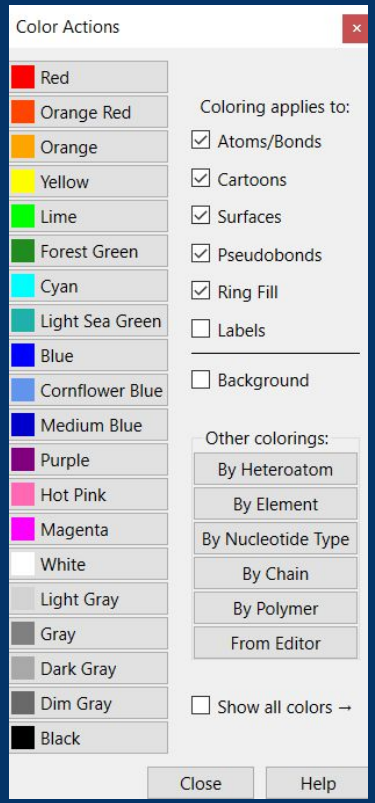
- I chose tube/slab style because I liked it



- Wanted to add color - but these don’t match Eterna!
  - Let’s do custom coloring

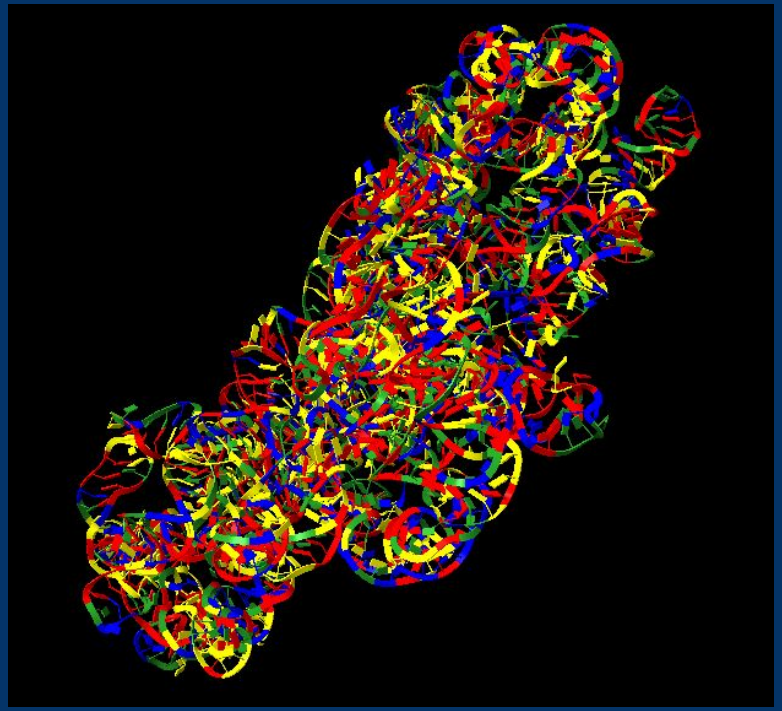
Using visual style options to better interpret 3D

- Go to Actions → Color → All Options to load color menu (keep this open)
- To assign the colors we want to the correct bases:
  - Go to Select → Residues → (your choice of residue)
    - The matching bases will highlight
  - Then click the color you'd like in the color menu
  - Repeat until all bases are colored as you wish
  - Then unselect everything (Select → Clear)



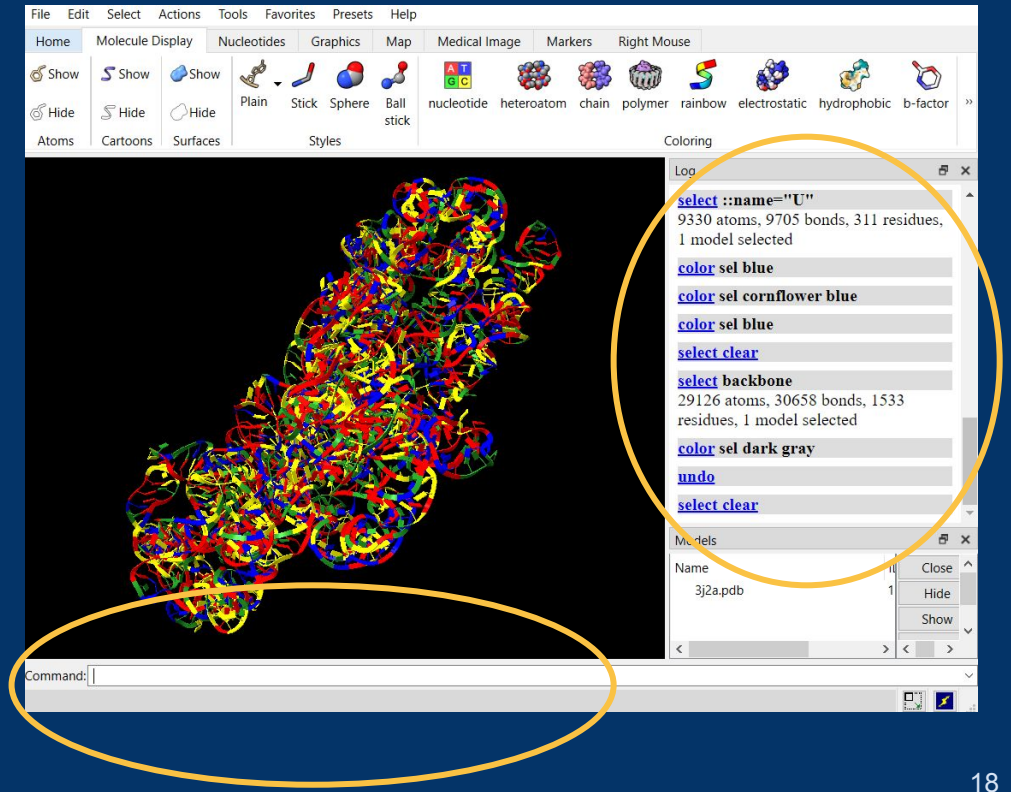
Using visual style options to better interpret 3D

- Colors should match with Eterna now!
  - Confirm by hovering over base until it tells you the identity



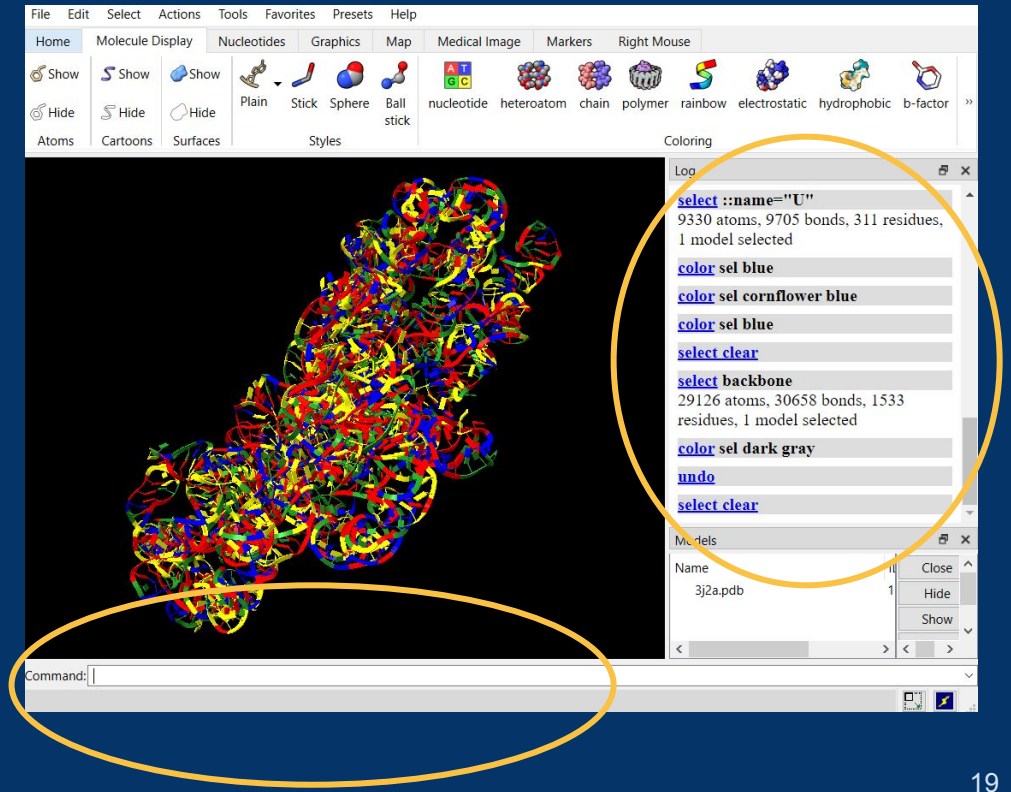
Using the command line

- I'd like to find base 744, which Nando was looking at
- I could find it by hand . . .
- . . . or I could use command line shortcuts to find it
  - Command line can be used for a lot
  - When you do an action using menus, ChimeraX also tells you what the corresponding text command would be
  - Useful command: undo (reverses previous action)



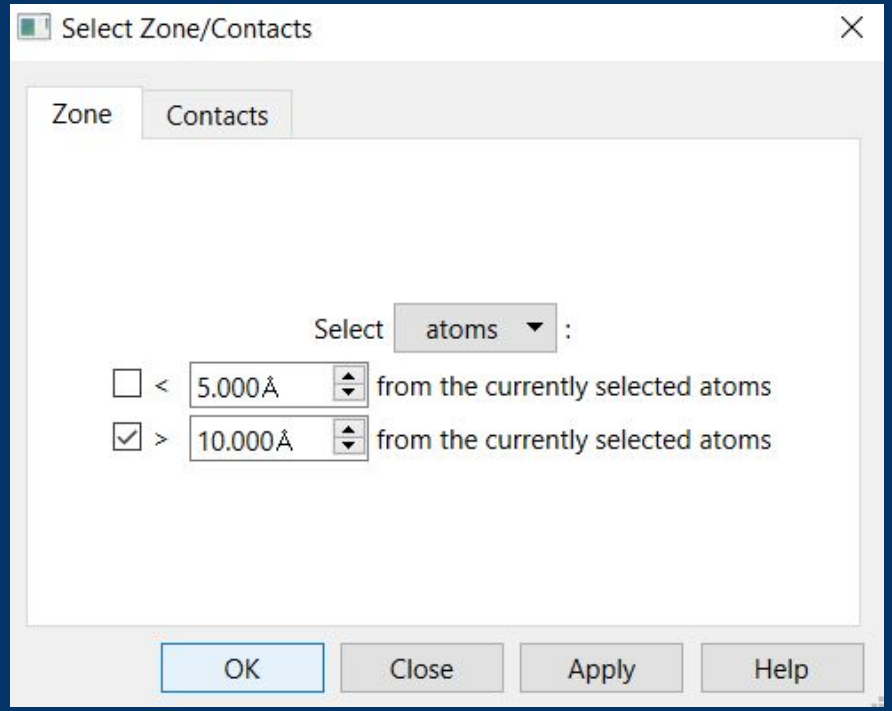
Using the command line

- Type the following into the command line and press enter:
  - sel :744
- “sel” is short for select
- The “:” tells us we’re looking for a base (also called a residue)



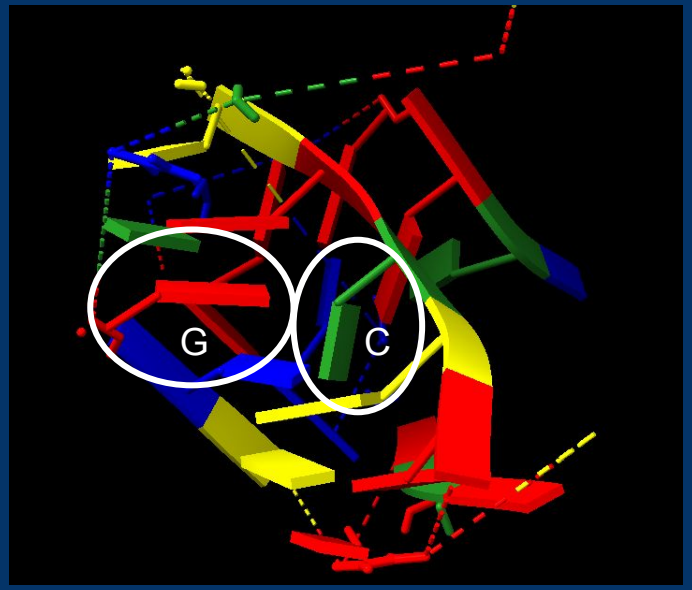
Focusing on a “zone”

- Still hard to find our base . . .
- Let’s select everything a certain distance away . . .
  - Select → Zone/Contacts → fill in the settings you’d like, then click OK
  - I chose > 10 Angstroms away
- . . . and delete it
  - “del sel” in command line
  - Maybe not the most elegant option, but works for my purposes
  - Feel free to use hiding, transparency, etc. if you prefer



Almost there . . .

- Much more manageable number of residues!
- After some rotation, I can see the bases Nando found (the G and C that weren’t pairing):

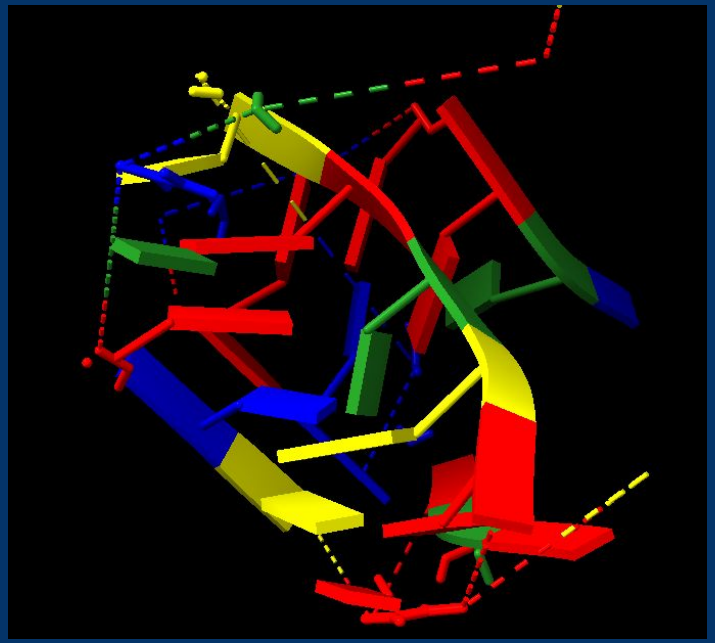


What are the (predicted) hydrogen bonds?

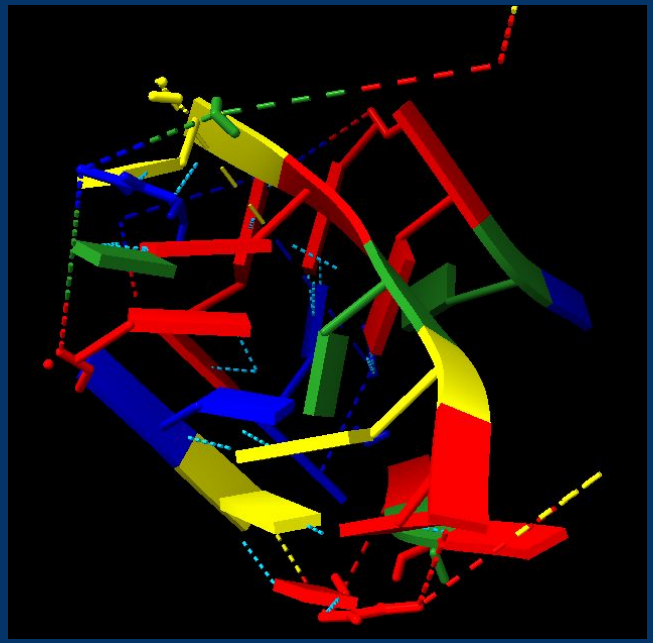
- Hydrogen bonding - the chemical interaction that causes base pairing (among other things)
  - Occurs when an electronegative atom, such as oxygen (O) or nitrogen (N), interacts with a hydrogen (H)
- We can visualize these interactions within ChimeraX
  - Type “hbond” in command line

What are the (predicted) hydrogen bonds?

Before visualizing hydrogen bonds

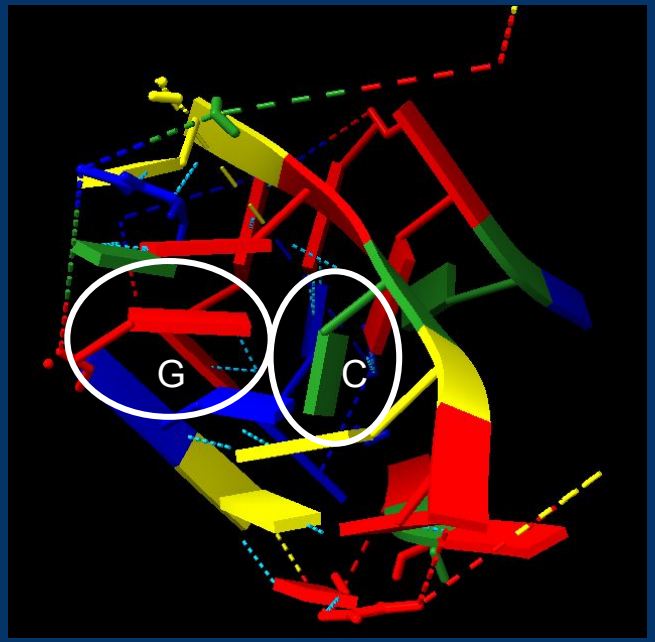


After visualizing hydrogen bonds



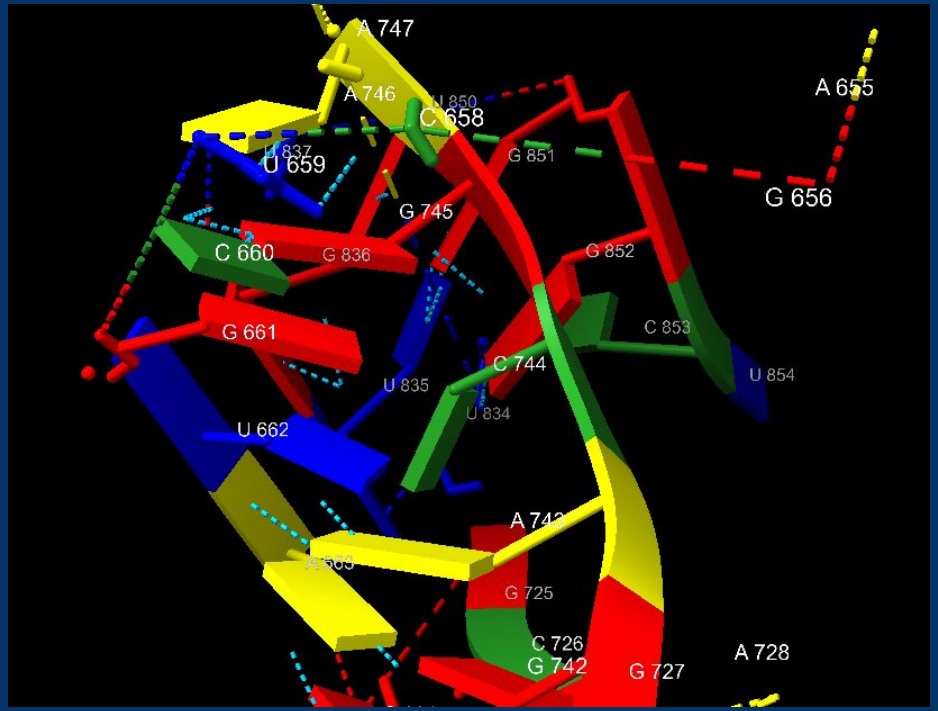
Mission accomplished!

- We understand why this G and this C do not pair together
- They don't pair together because they don't have the right "shape" (angle, distance) to hydrogen bond
- Along the way, we learned some basics of how to use ChimeraX
  - Visual settings
  - Using the command line
  - Isolating a zone of interest
  - Visualizing hydrogen bonds



Just one more thing . . .

- Adding labels!
- To get this picture, I did the following:
  - Actions → Label → Residues → Name and Number
- Good to see it's the correct base!



More guides for Chimera(X)

- Introduction to Chimera for EteRNA Players by Omei and Eli
- Bare Bones Guide to Creating 3D-RNA Structure Models Using UCSFs Chimera by AndrewKae
- ChimeraX Quick Start Guide (provided by ChimeraX)
- Command-Line Target Specification documentation (provided by ChimeraX)
  - Useful for complicated structure files - for examples, ones with multiple RNAs
  - Also useful for knowing how to select individual atoms, etc.

Questions?