

Immersive Visualization of Proteins in Virtual Reality with ChimeraX

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Structure is FUN!!



Agenda

- How to put on a headset; use of controllers
- Intro VR session- Hemagglutinin 5UGY
 - Influenza hemagglutinin in complex with a neutralizing antibody
- VR basics
 - Controllers
 - Hardware
- Introduction to Computational Structural Biology
 - Drug Discovery/Design
 - Review of Protein Chemical Structure
 - Primary, Secondary, Tertiary, Quaternary Structure
- Introduction to Structure Databases: Protein Data Bank
- ChimeraX Basics
 - Controls, screens, obtaining structures, representations, colors labels, selection
- Hands on session #1: Create “Review of Protein Chemical Structure” scenes
 - Build, color, add hydrogens, add labels, save session and image files

- Hands on session #2: Set up the Hemagglutinin VR session (PDB 5UGY)
 - Fetch, representations, deleting atoms, more colors, surfaces, interaction interfaces , zone selection
- Hands on session #3: Plasmodium Dihydrofolate Reductase- PDB entry 4DPD
 - Fetch, delete chains, highlight ligand, add labels, surfaces and transparency, zone selection
 - H-bonds and contacts, Sequence Viewer, aligning structures with Matchmaker
 - Save in .glb format
- Adding a live view into your presentations
- Back to VR: 4DPD session

Extras:

- Bonus exercise 1: LookSee: VR without computer
 - 3D graphics vs. Chemical graphics
 - Scene triangle adjustments
- Bonus exercise 2: Pathogen AR- Augmented Reality Phone App
- Bonus #3: NIH 3D WebXR

UCSF ChimeraX

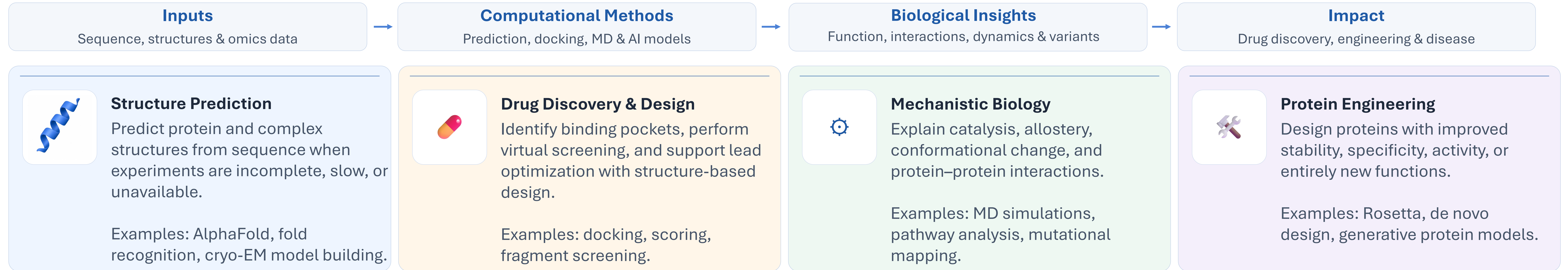
- UCSF Chimera/ChimeraX
 - Free
 - Easy to use
 - Multiplatform: Windows, Mac Linux
 - ⁴ VR capability (Windows only)
 - Graphical interface and command line
 - Close integration with AlphaFold
 - Fitting CryoEM density maps to protein structures
 - Medical imaging

Download from:

<https://www.rbvi.ucsf.edu/chimerax/download.html>

Computational Structural Biology

Transforming Molecular Structure into Biological Discovery



Sequence → Structure → Dynamics → Function → Therapeutic & Scientific Impact

Scope of the Drug Discovery/Design Problem

Total number of compounds available for screening in a large Pharma library $\sim 10^6 - 10^7$

Total number of possible "drug-like" molecules (chemistry space) $\sim 10^{60} - 10^{90}$



Chris Lipinski

What is a "drug-like" molecule?

Lipinski's "Rule of 5"

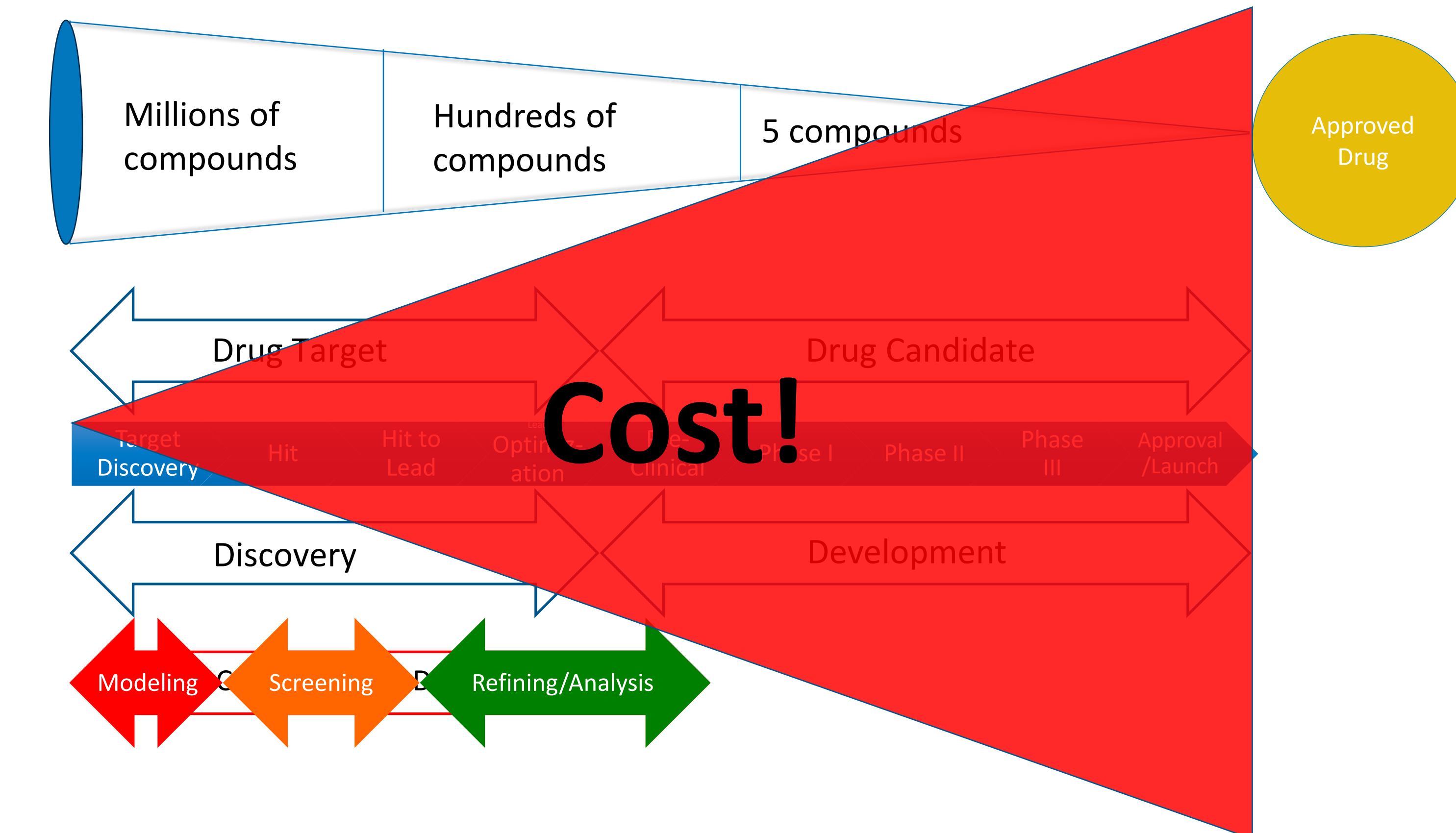
< 5 H-bond donors

< 10 H-bond acceptors

molecular weight < 500 g/mol

partition coefficient ($\log P$) < 5

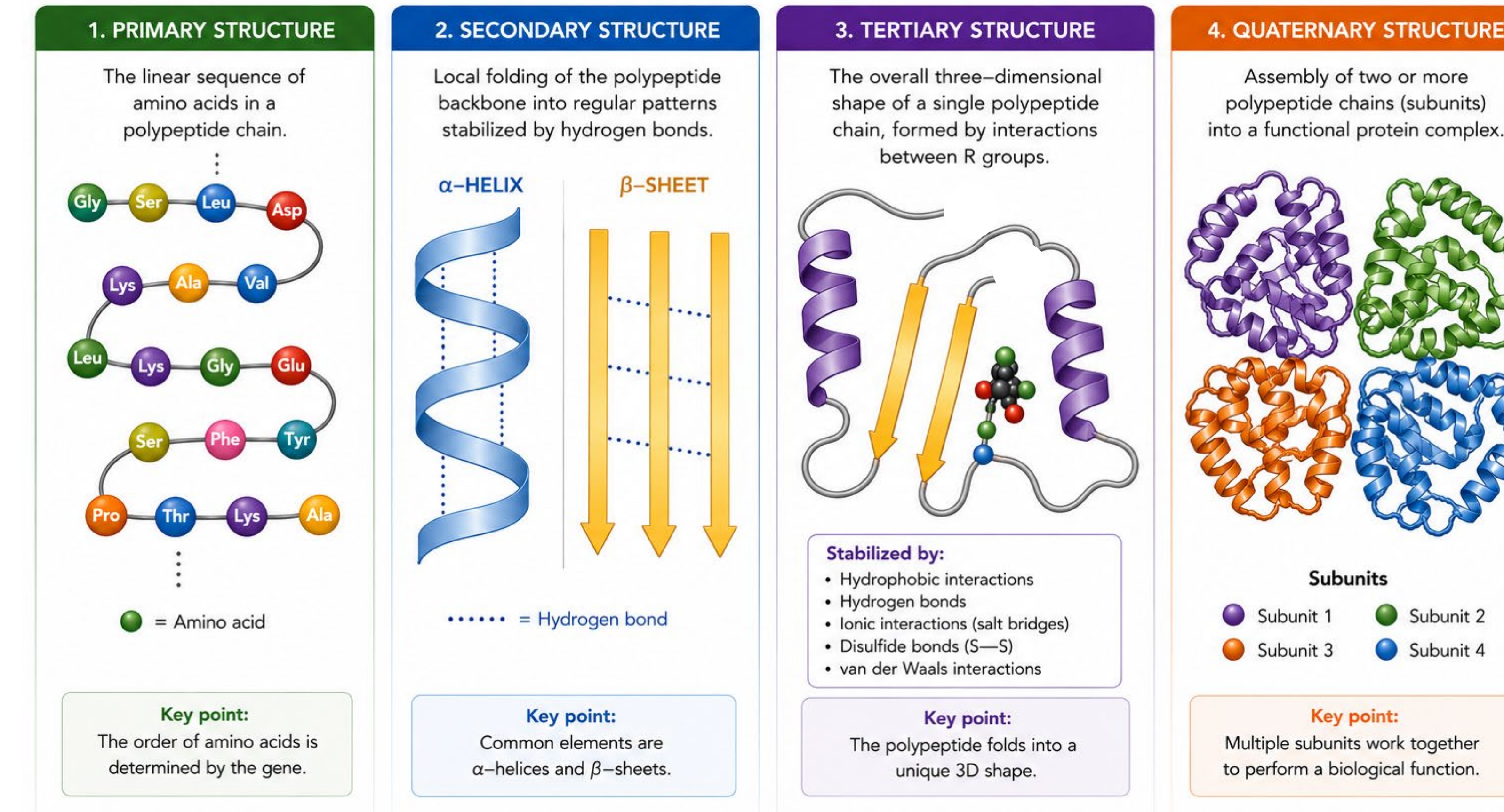
Drug Creation Process



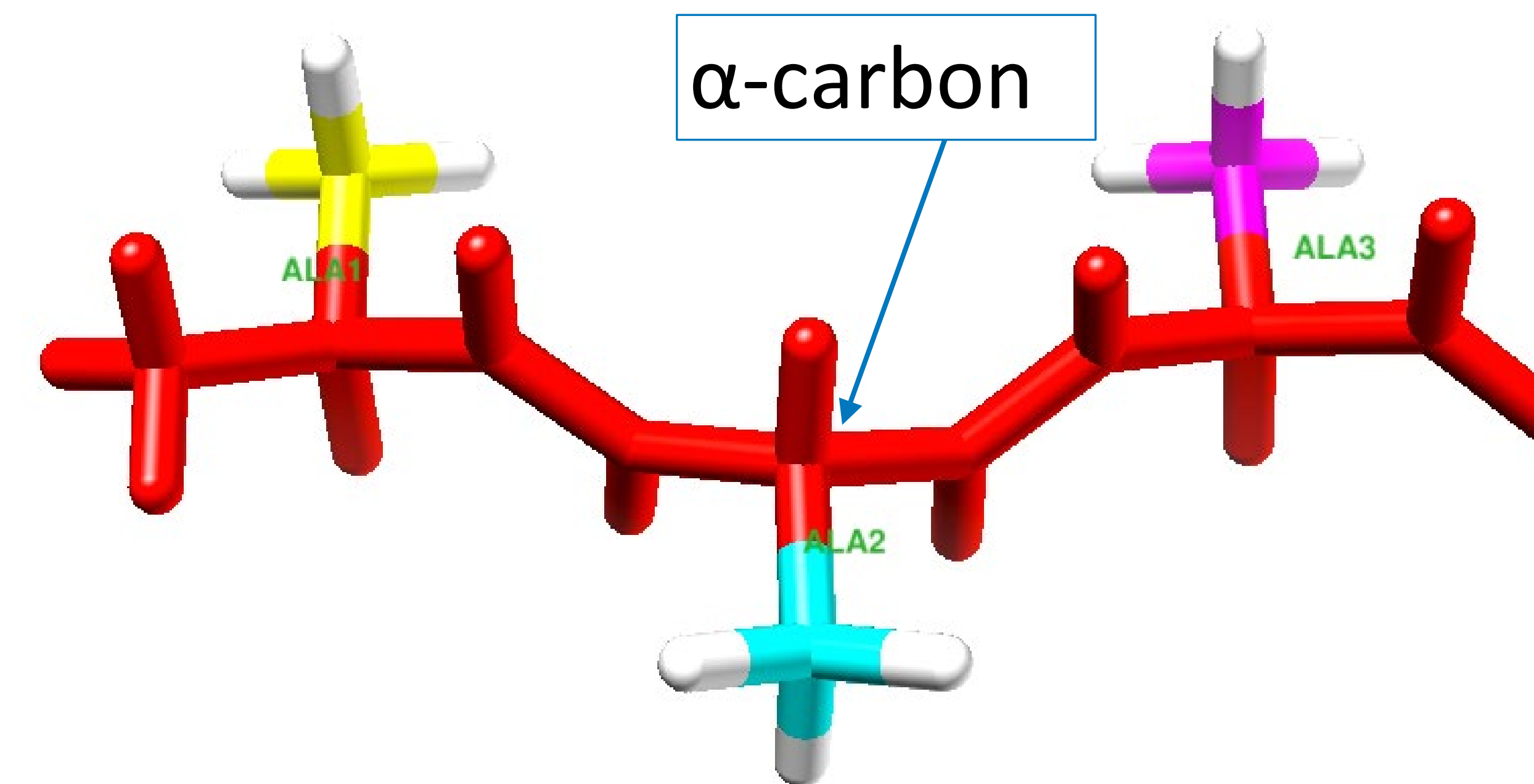
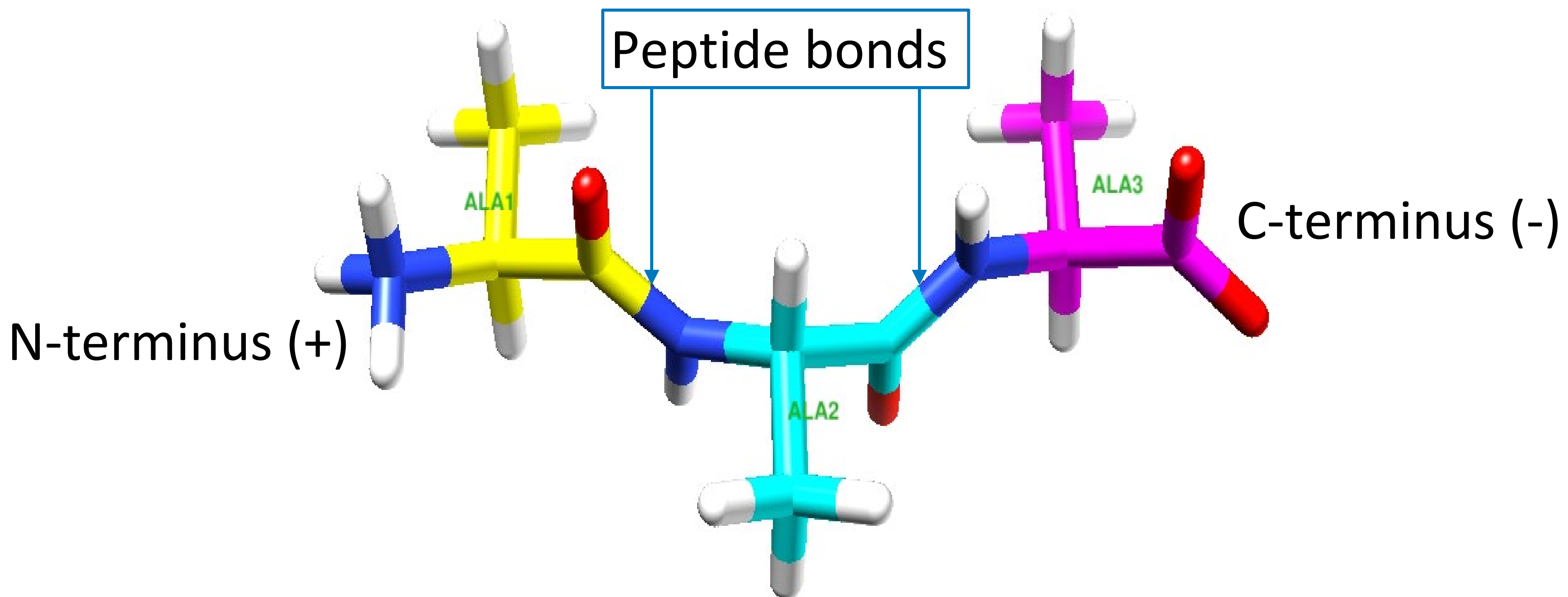
Protein Structure

Levels of Protein Structure

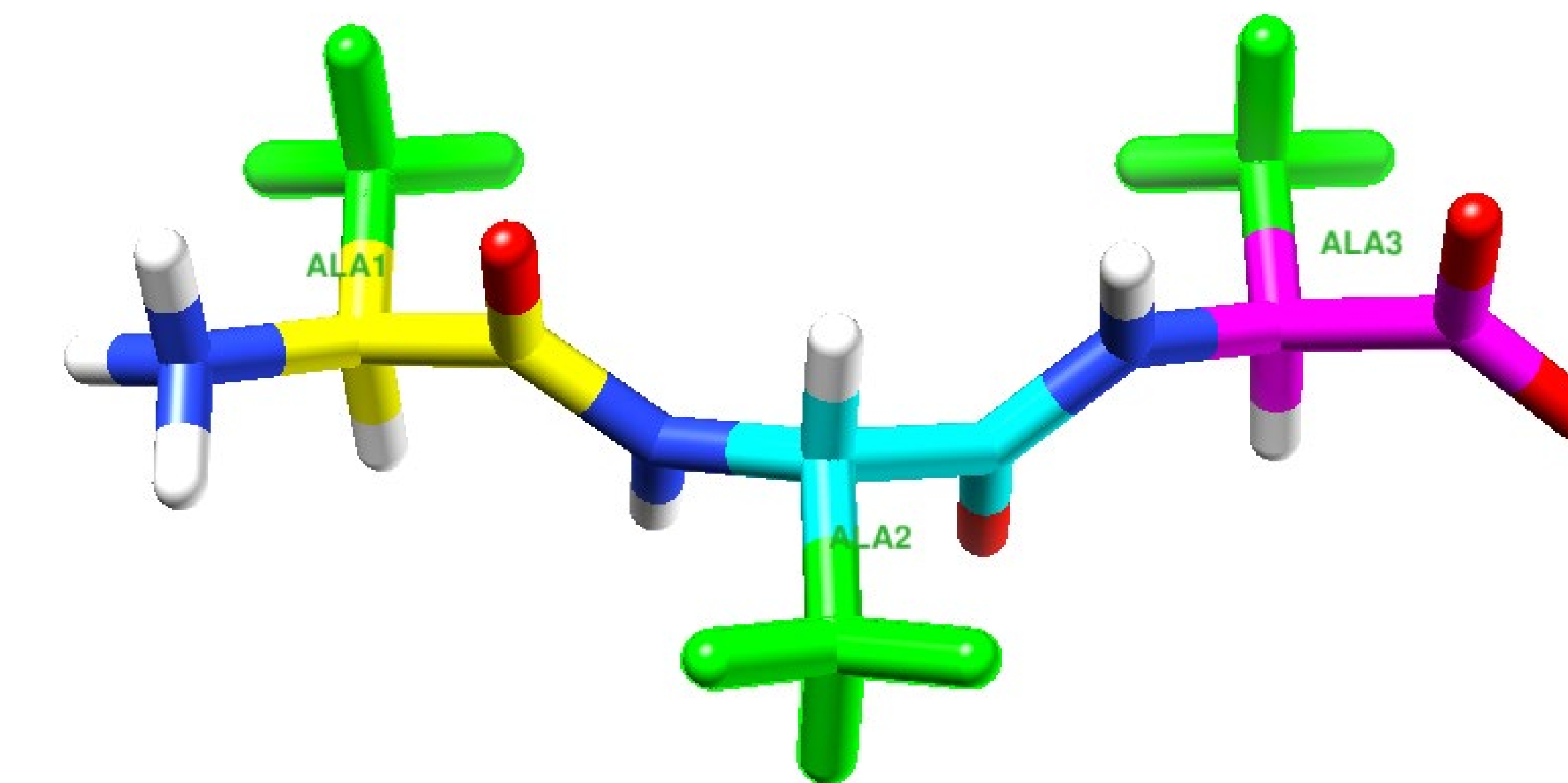
Proteins are hierarchical molecules with four levels of structure.



Quick Review of Protein Chemical Structure

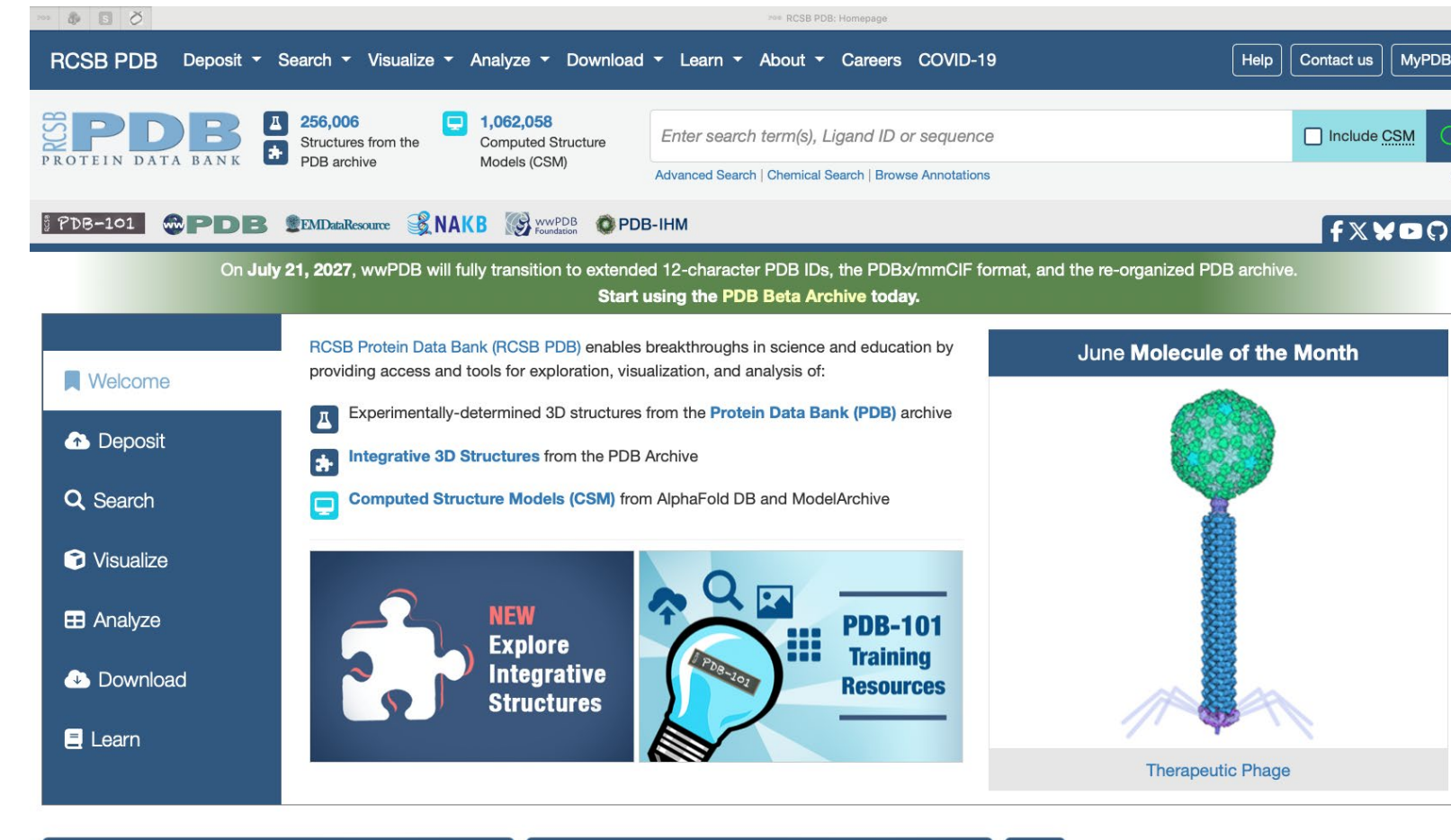


Backbone



Sidechains

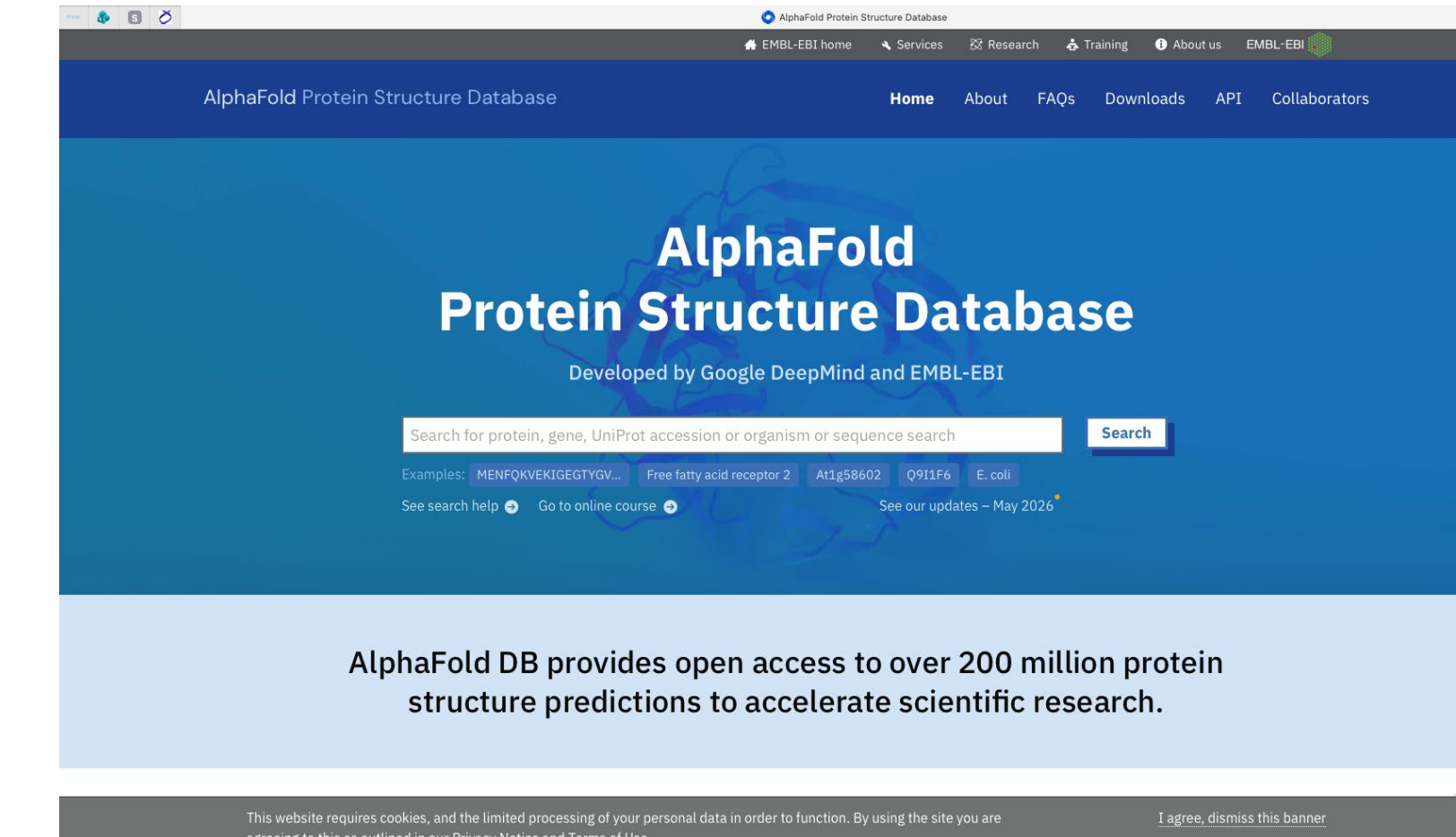
Some sources of Protein Structures



RCSB PDB- <https://www.rcsb.org>

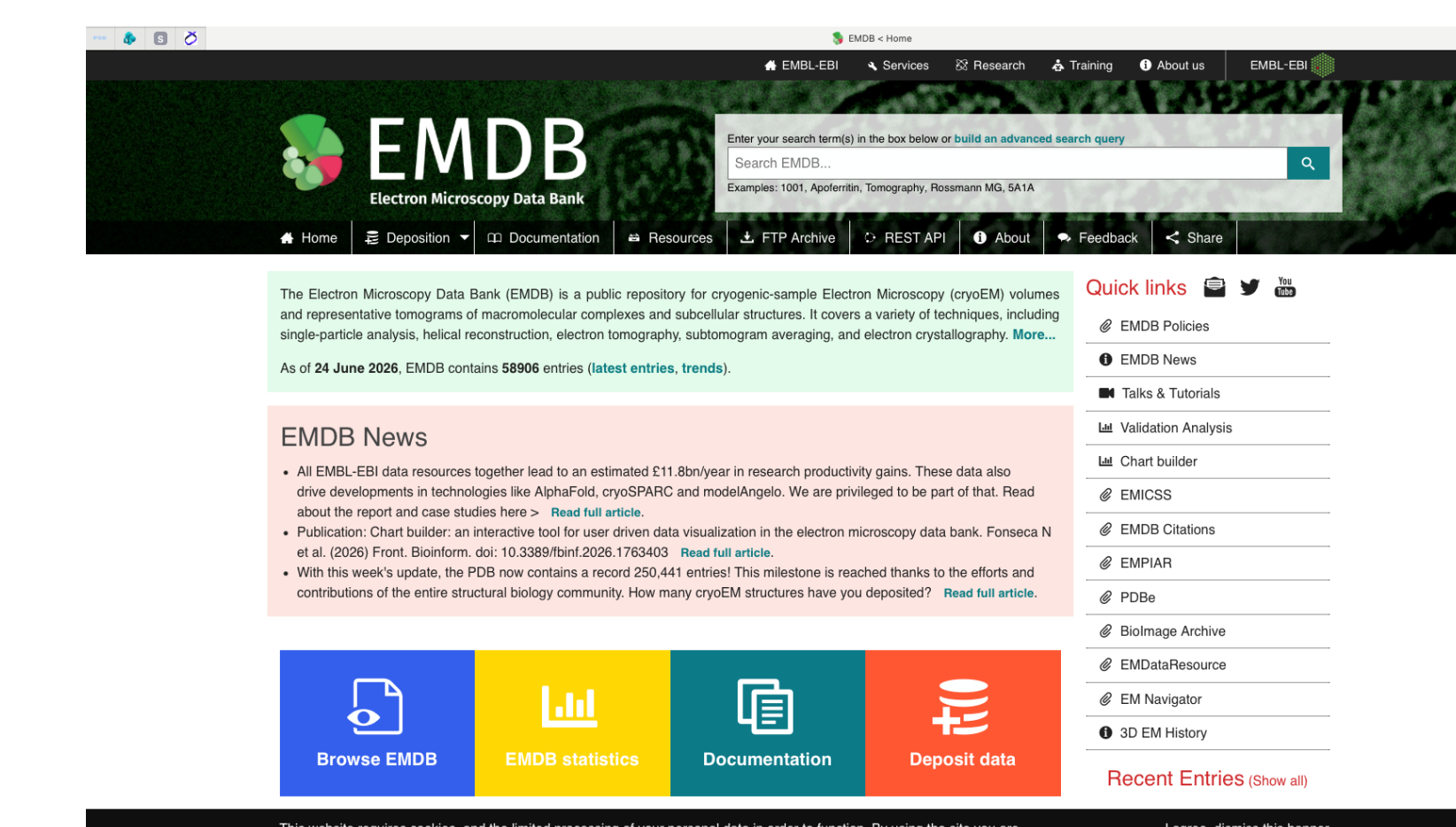
Experimental atomic structures:

Mostly from X-ray, CryoEM, and NMR



AlphaFold- <https://alphafold.ebi.ac.uk>

Structure predictions from AlphaFold2

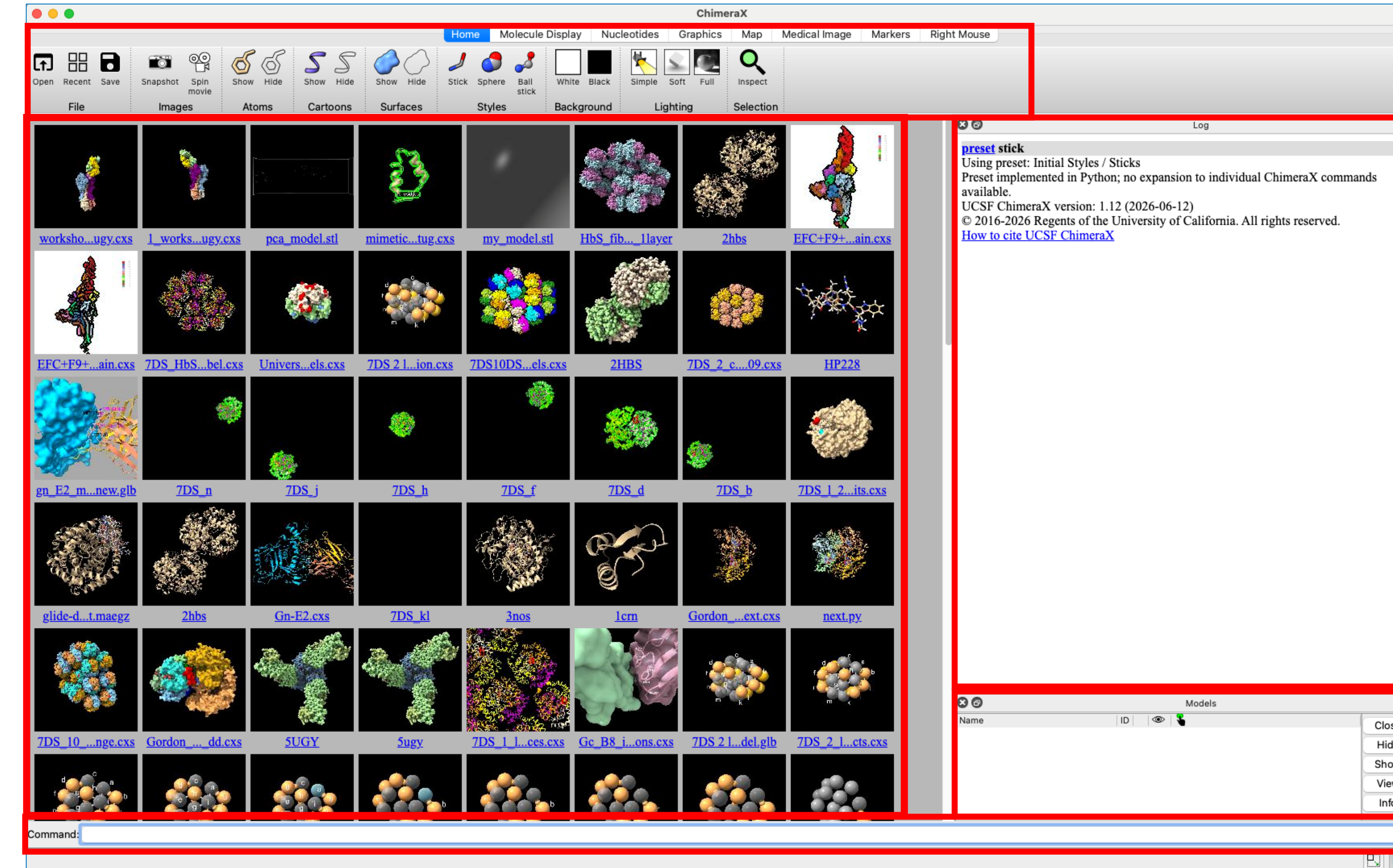


EMDB: <https://www.ebi.ac.uk/emdb/>

Electron Microscopy Data Bank

Processed 3D volumes and tomograms

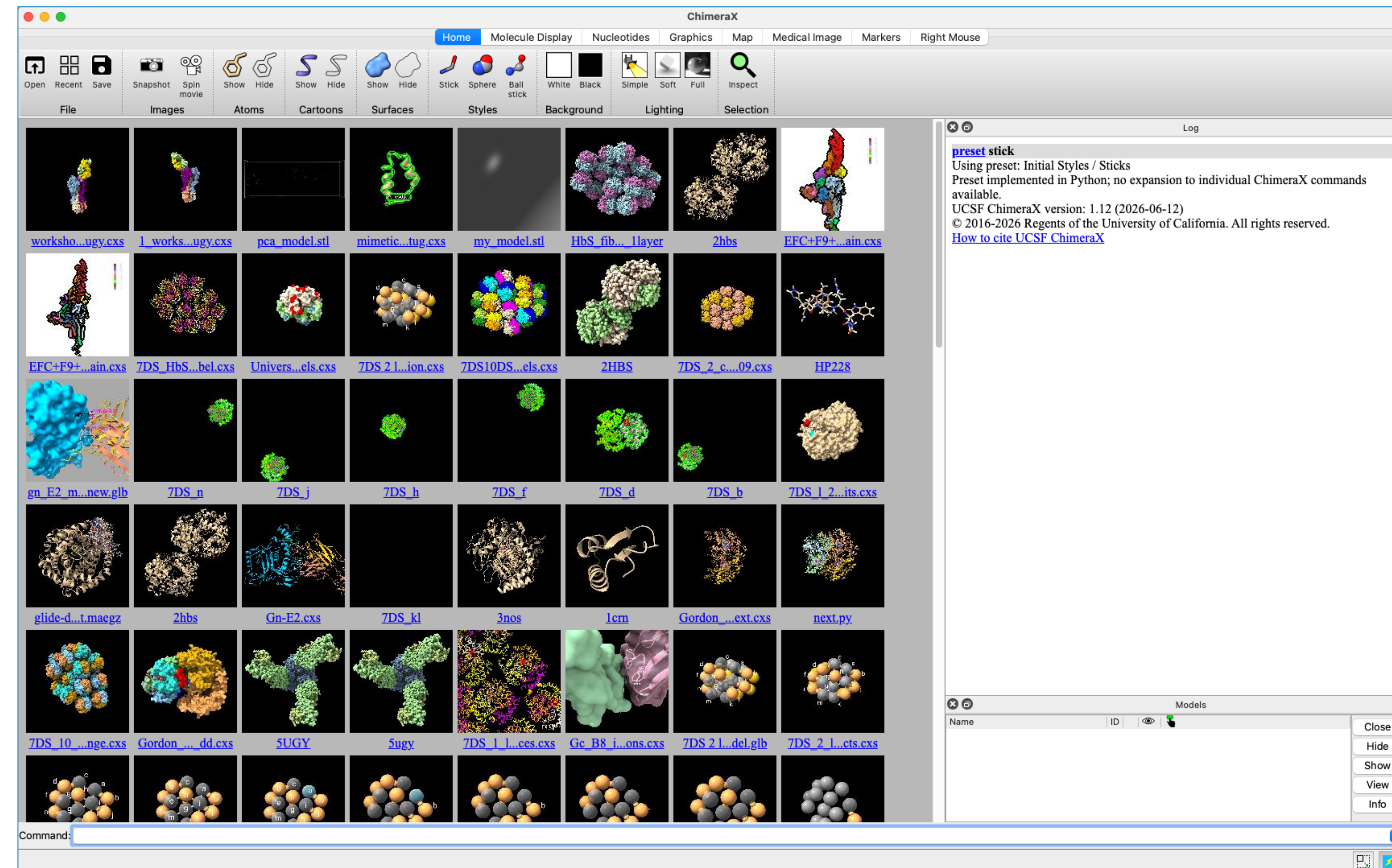
UCSF ChimeraX- Overview



Navigating ChimeraX

1. Menubar
2. Main Graphics Window
Session History at Startup
3. Tabs/Toolbar Icons
4. Log
5. Command Line
6. Model Panel

ChimeraX- Exercise 1: Create “review of protein structure” scenes



Build the AlaAlaAla peptide:

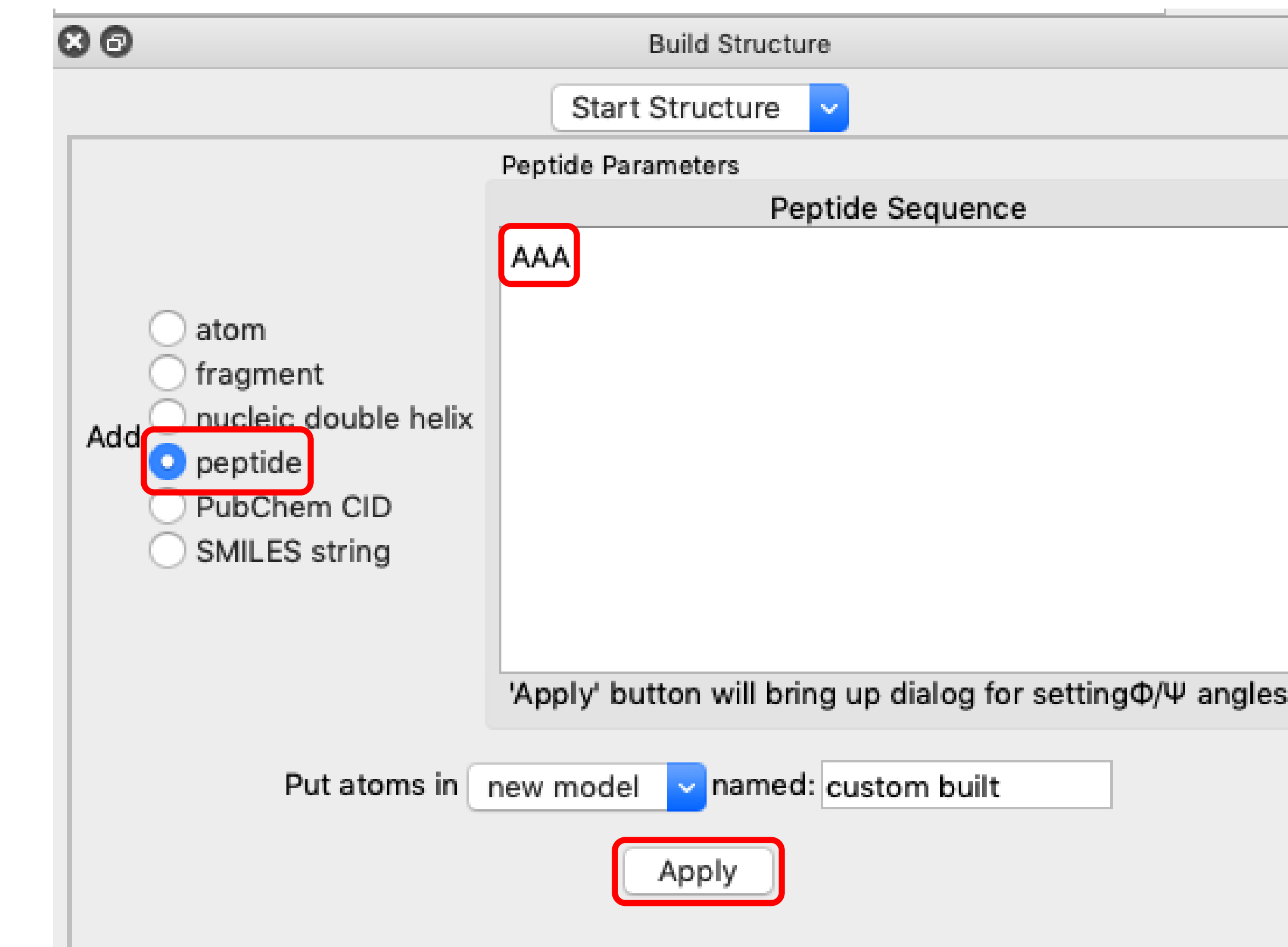
1. Tools>>Structure Editing>>Build Structure

Within the dialog box:

2. Choose Add “peptide”

3. Enter "AAA" in the Peptide Sequence field

4. Click “Apply”



Build an AlaAlaAla peptide (continued):

1. Select all three rows in the dialog box that appears
2. In “Seed above Phi/Psi with values for:” choose "antiparallel β strand”
3. Click "Set", then OK
4. Click the “x” to remove the “Build Structure” dialog

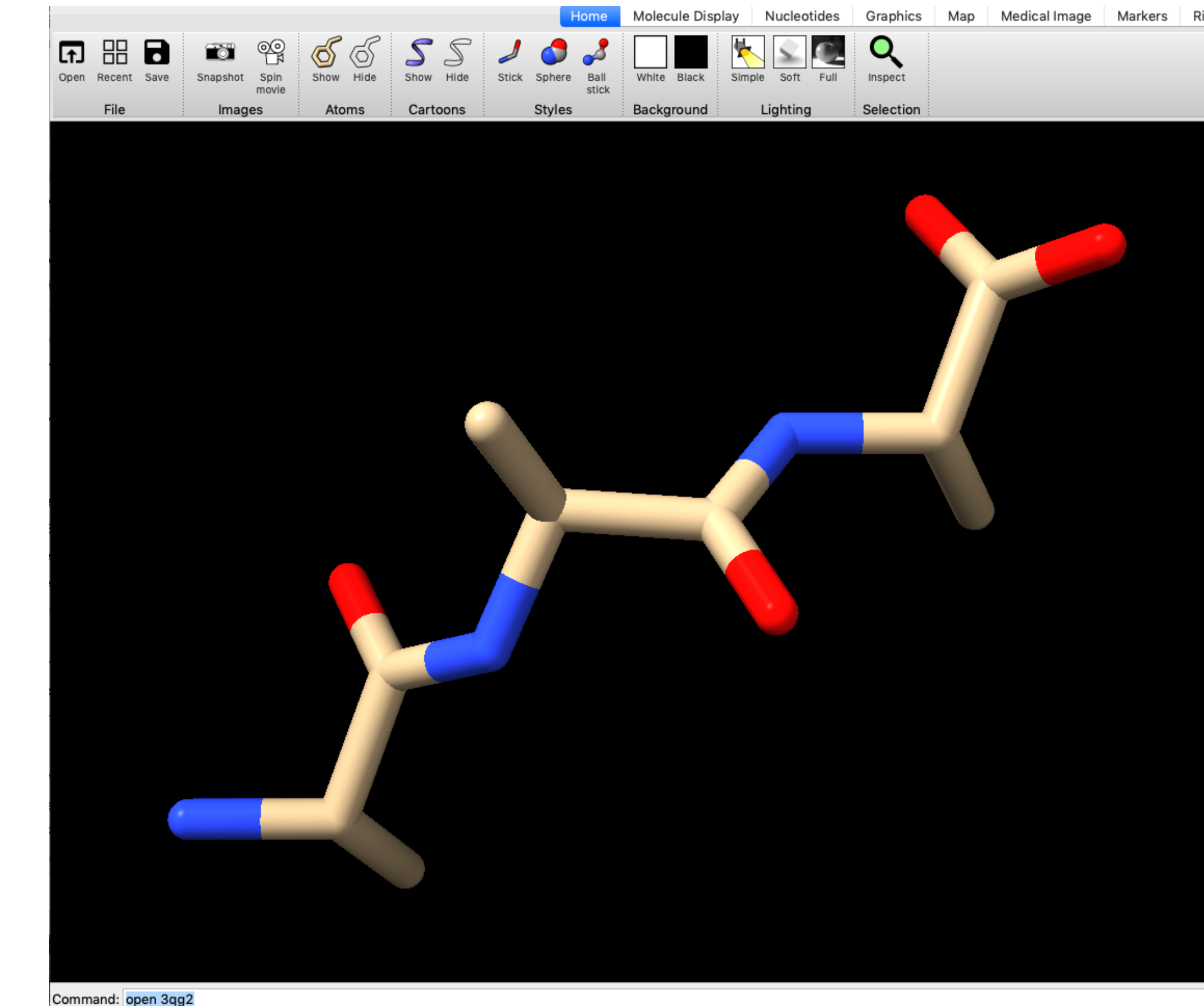
Res	Φ	Ψ
A	-139	135
A	-139	135
A	-139	135

Set selected rows to Φ : -139 Ψ : 135

Seed above Φ/Ψ with values for: antiparallel β strand

Rotamer library: Dunbrack chain ID: auto

Cancel OK



Adjust the background; add Hydrogen atoms

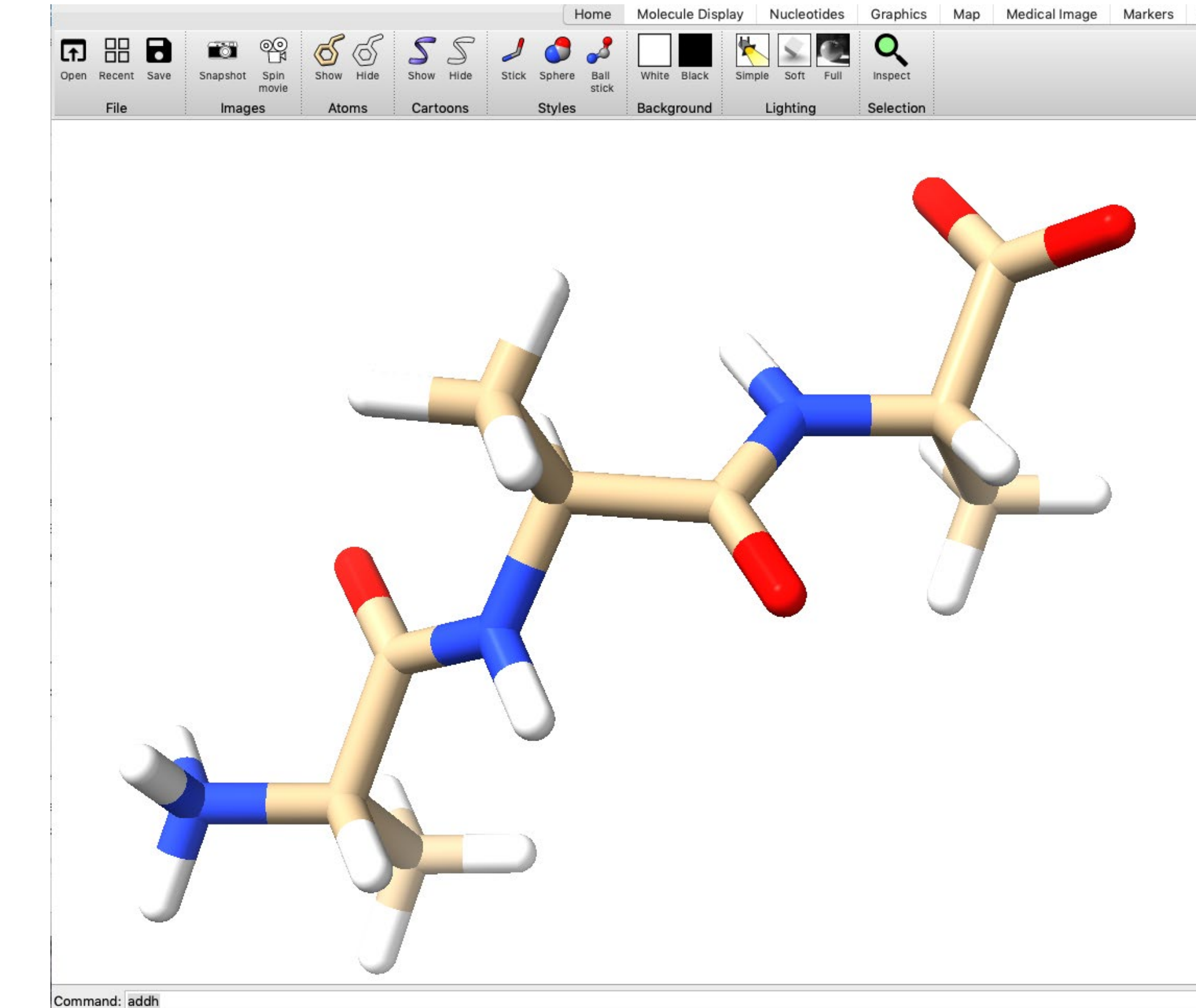
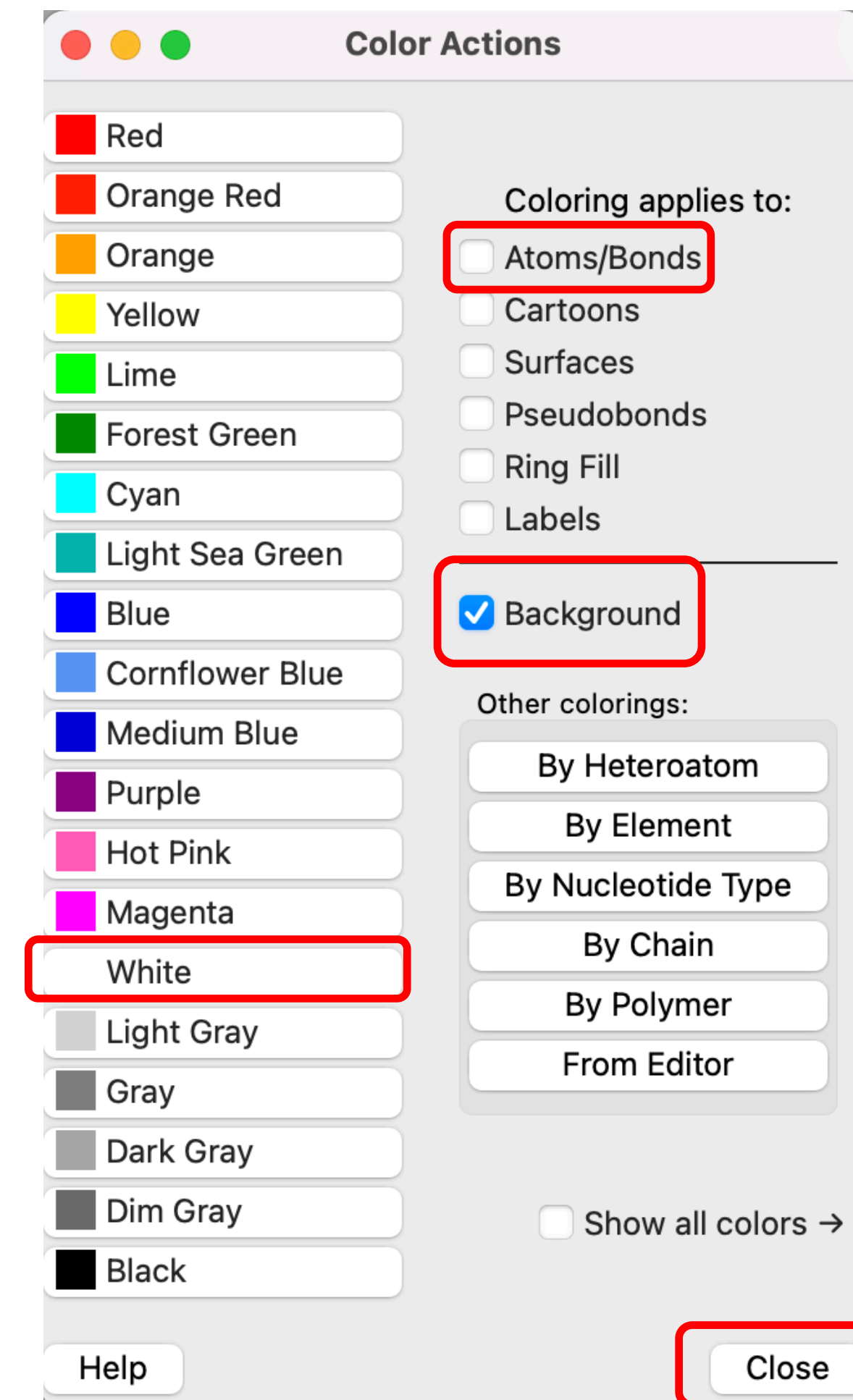
1. Actions>>Color>all options...>>

2. In the Color Actions dialog box:
Click “background” then choose white

3. In the “Coloring applies to:” section:
Click “atoms/bonds”
Click “Close”

4. In the command line at the bottom of
the window type the command to add
hydrogen atoms:

addh



ChimeraX Mouse Controls

Use mouse controls to match the scene with the image at right:

Mouse buttons

Left: Rotate x or y

(with cursor in corner- rotate z)

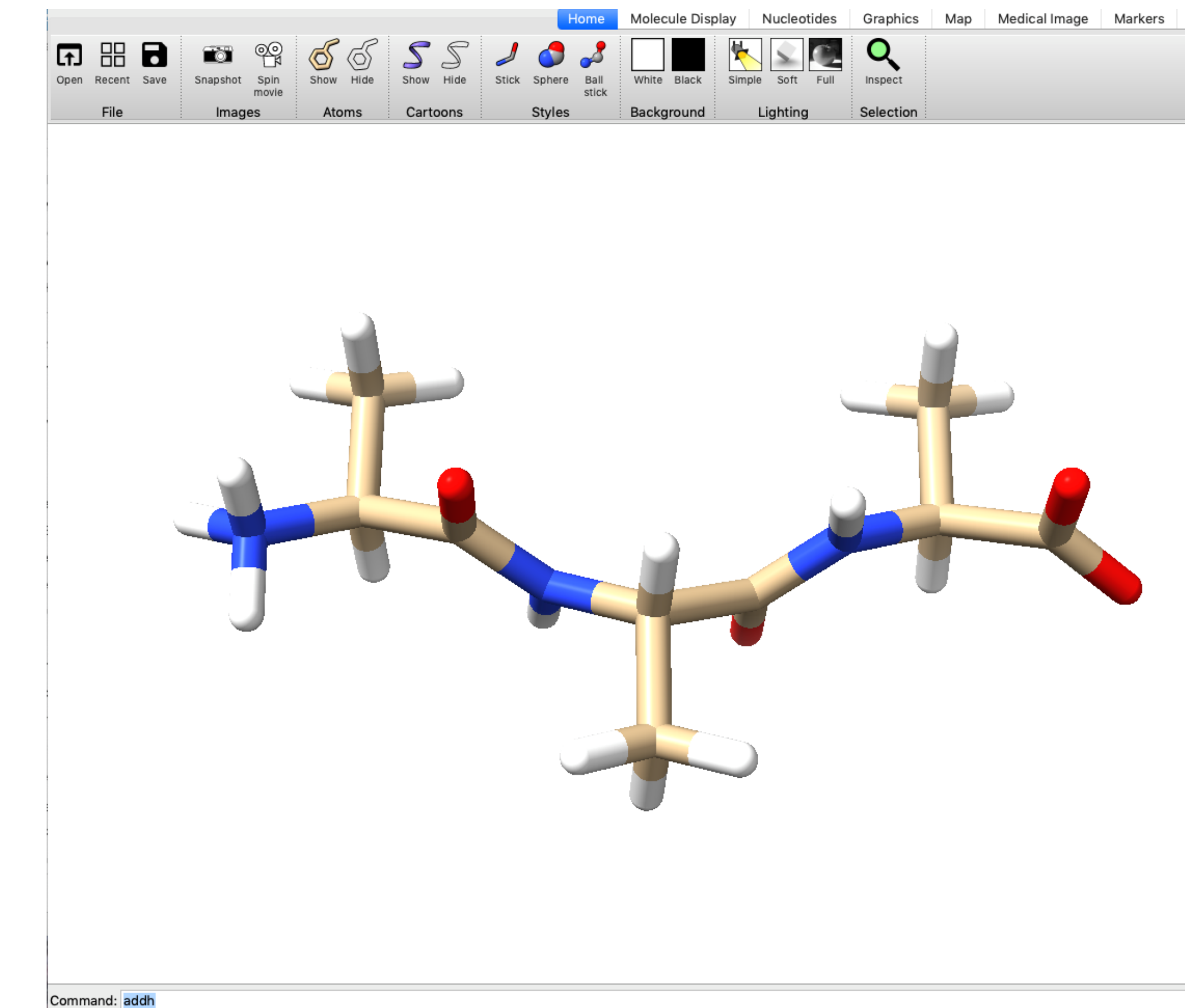
Middle: Translate

Right: Assign to an action from the “Right Mouse” tab

Mouse wheel: Resize

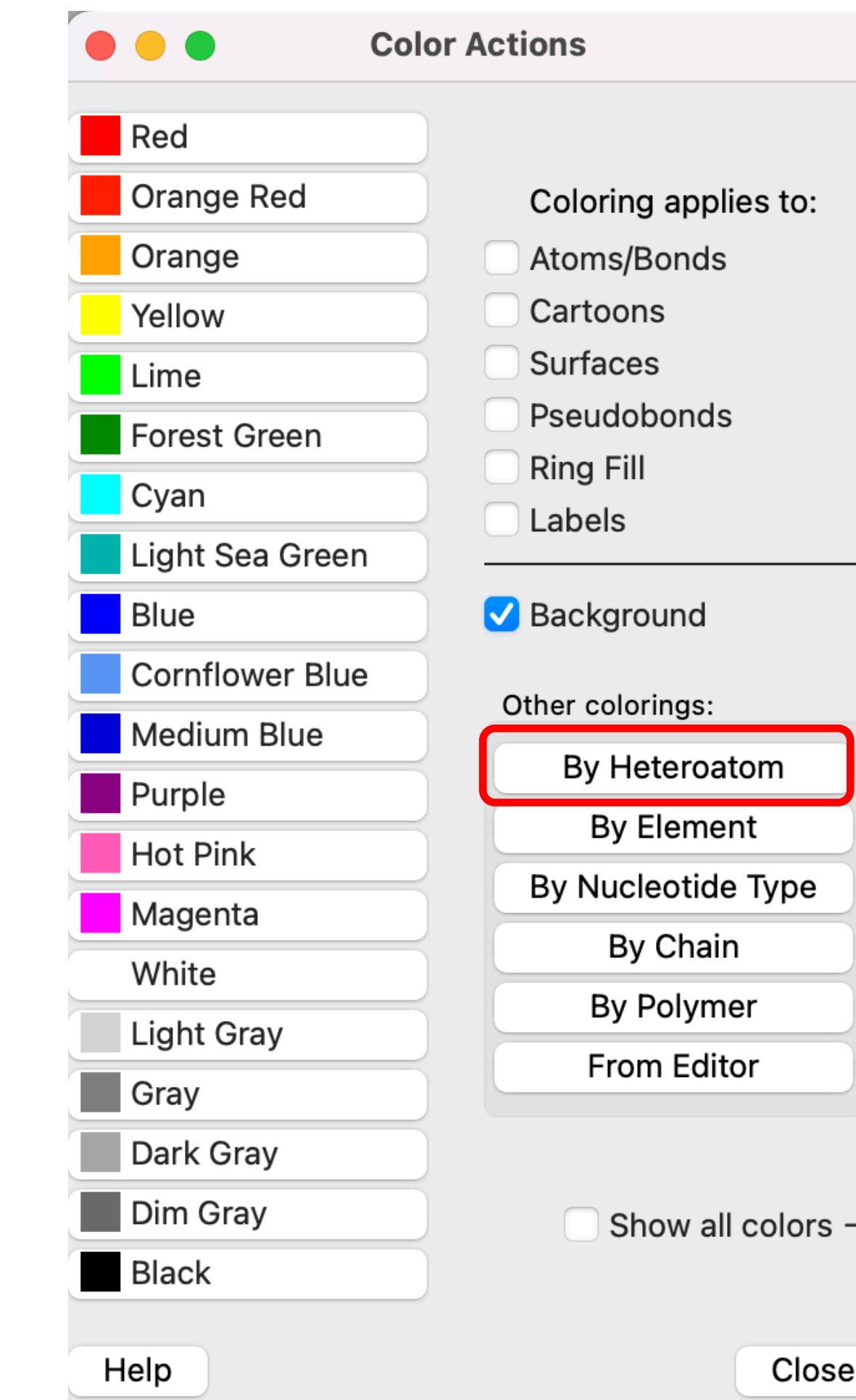
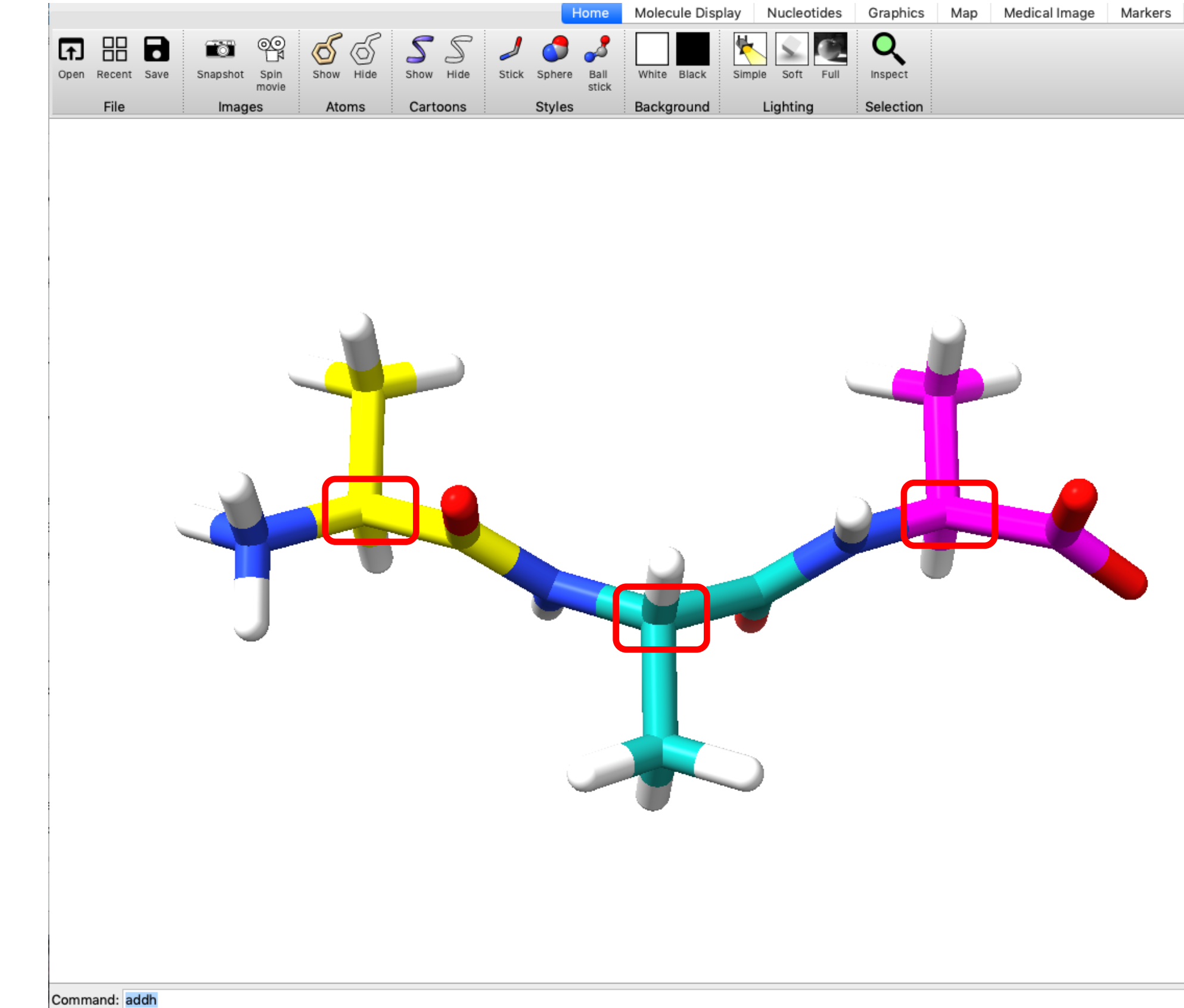
Control-Left-click: Select

(clicking in backdrop clears selection)



Color the residues

1. Control-click on the left-most alpha-carbon to select it.
2. Press the up arrow to select the entire amino acid.
3. Actions>>Color>>yellow
4. Control-click on the middle alpha-carbon to select it.
5. Press the up arrow to select the entire amino acid.
6. Actions>>Color>>cyan
7. Control-click on the right-most alpha-carbon to select it.
8. Press the up arrow to select the entire amino acid.
9. Actions>>Color>>magenta
10. Select>>Clear (or control-click away from any atoms)
11. Actions>>Color>>by heteroatom



Add labels

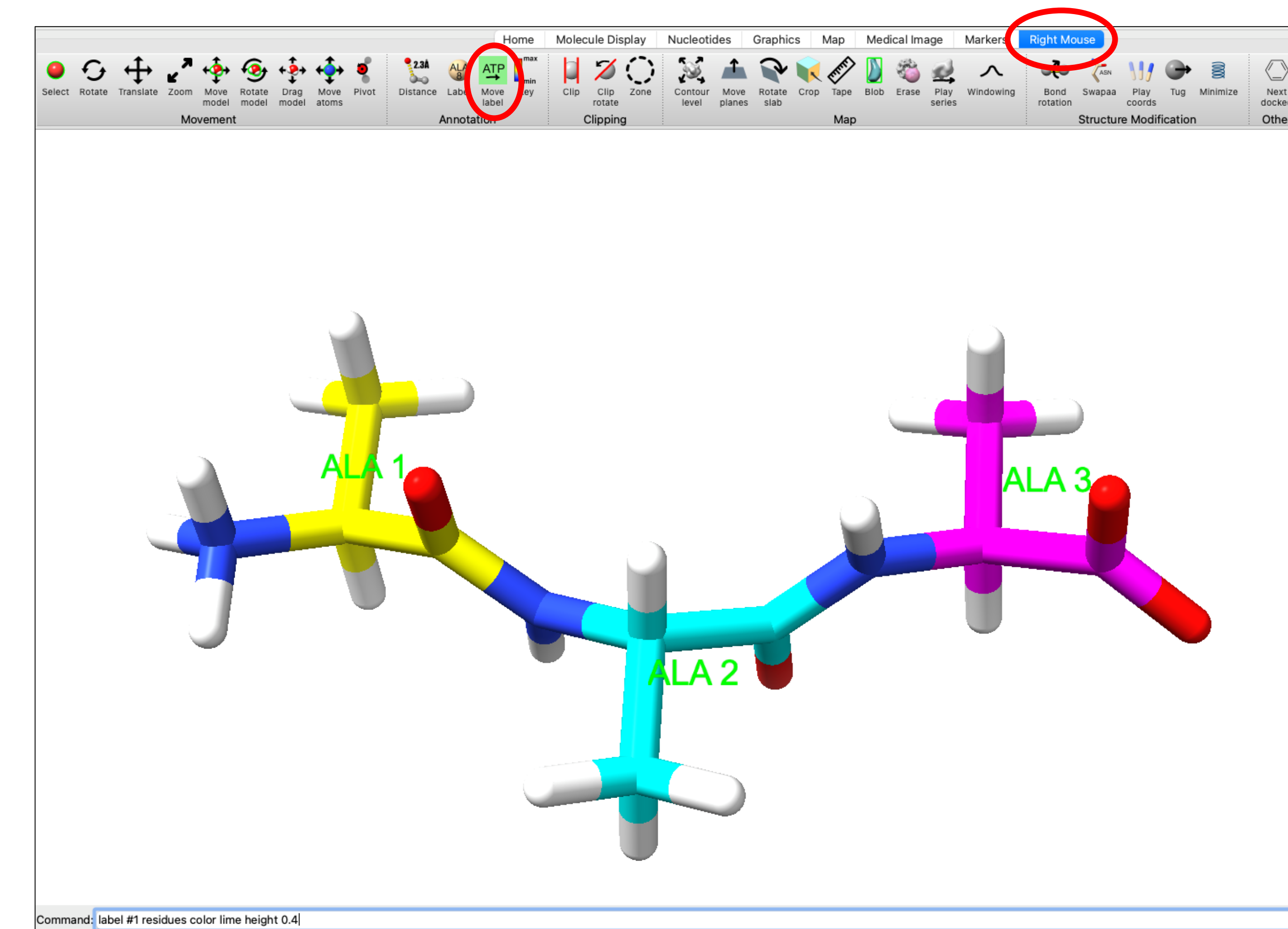
1. In the command line type:

label #1 residues color lime height 0.4

2. To precisely move a label, click the "Right Mouse" tab at the top of the screen, then left-click the "Move label" icon:



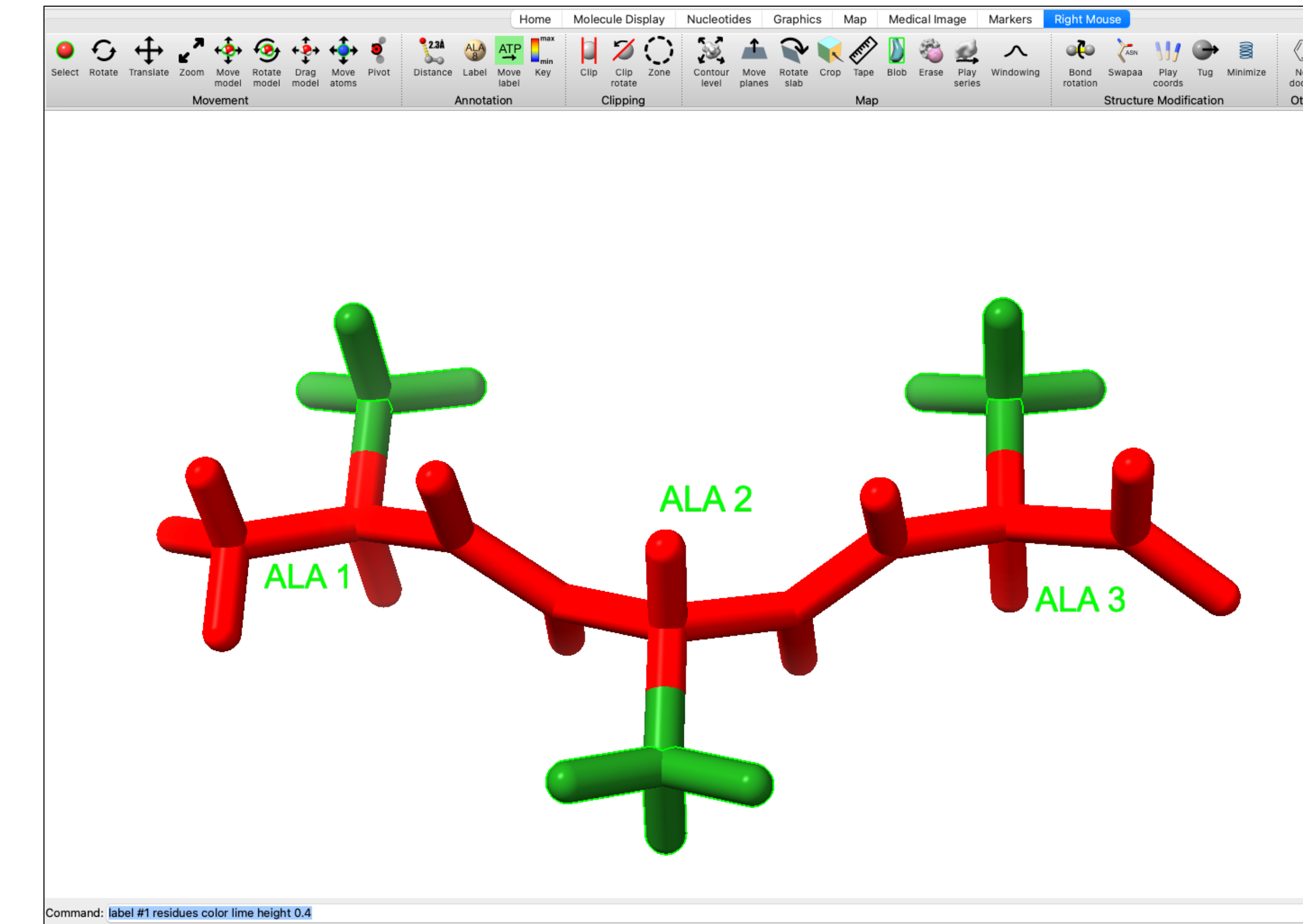
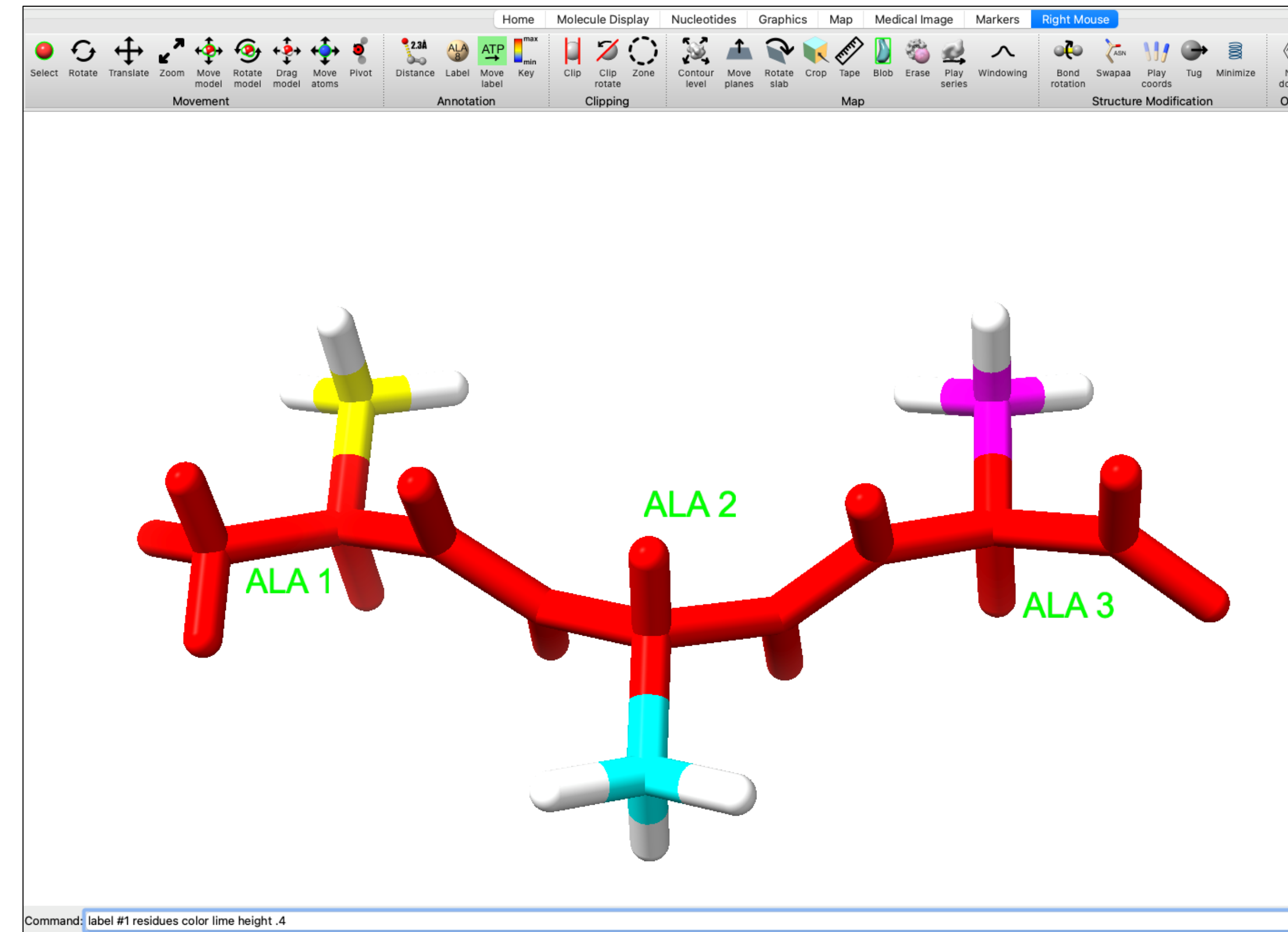
Now you can move labels by clicking on them with the Right Mouse button.



Color backbone red and side chains green

1. Select>>Structure>>Backbone
2. Actions>>Color>>Red
3. Select>>Clear to clear the selection
4. Select>>Structure>>sidechain Only
5. Actions>>Color>>Forest Green

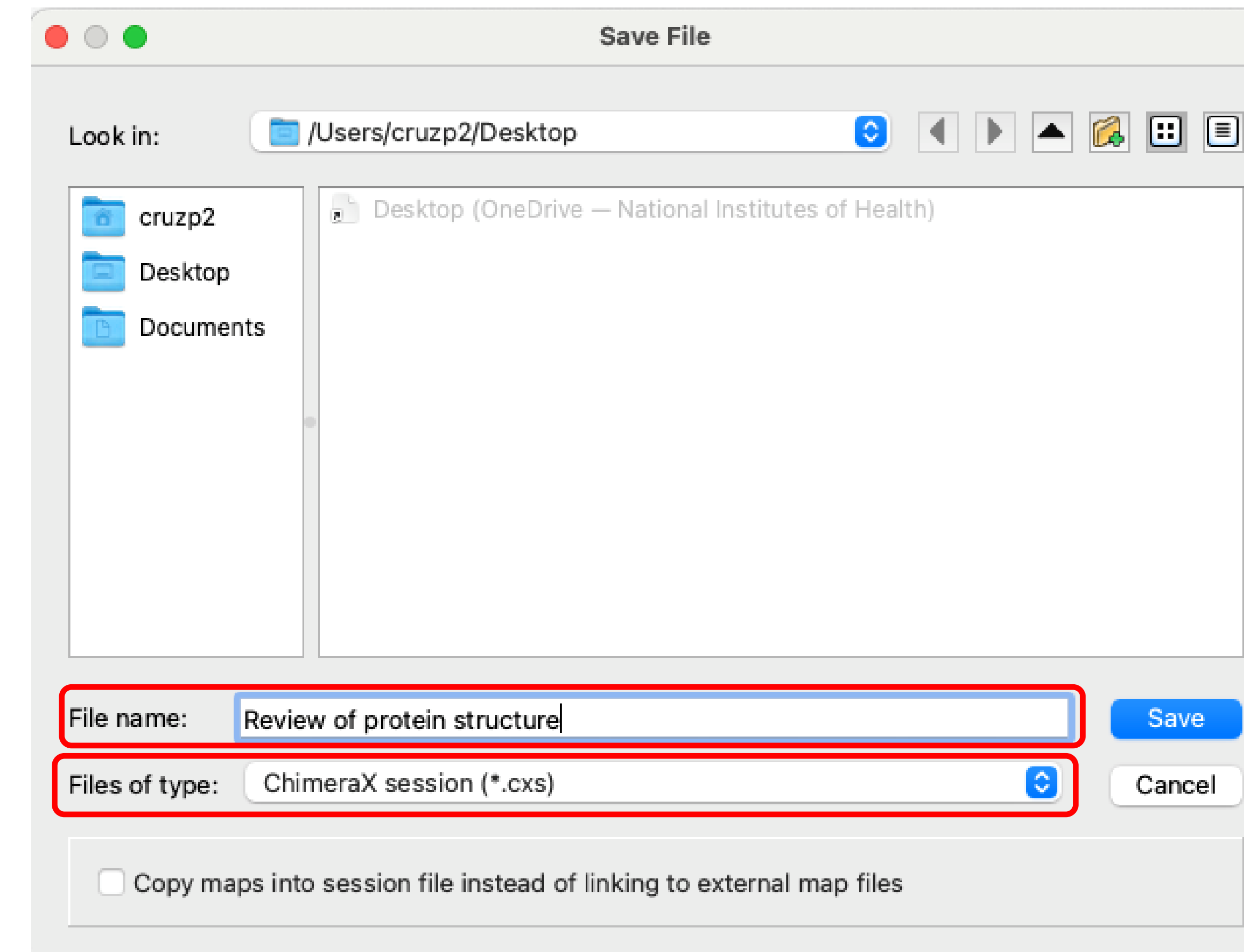
See if you can figure out how to get the backbone colors back and only color the sidechains.



Save the current scene

Save as a ChimeraX session file

1. File>>Save
2. In “Files of type:” choose:
ChimeraX session (*.cxs)
3. Enter a file name, for example:
Review of protein structure
4. Click “Save”.

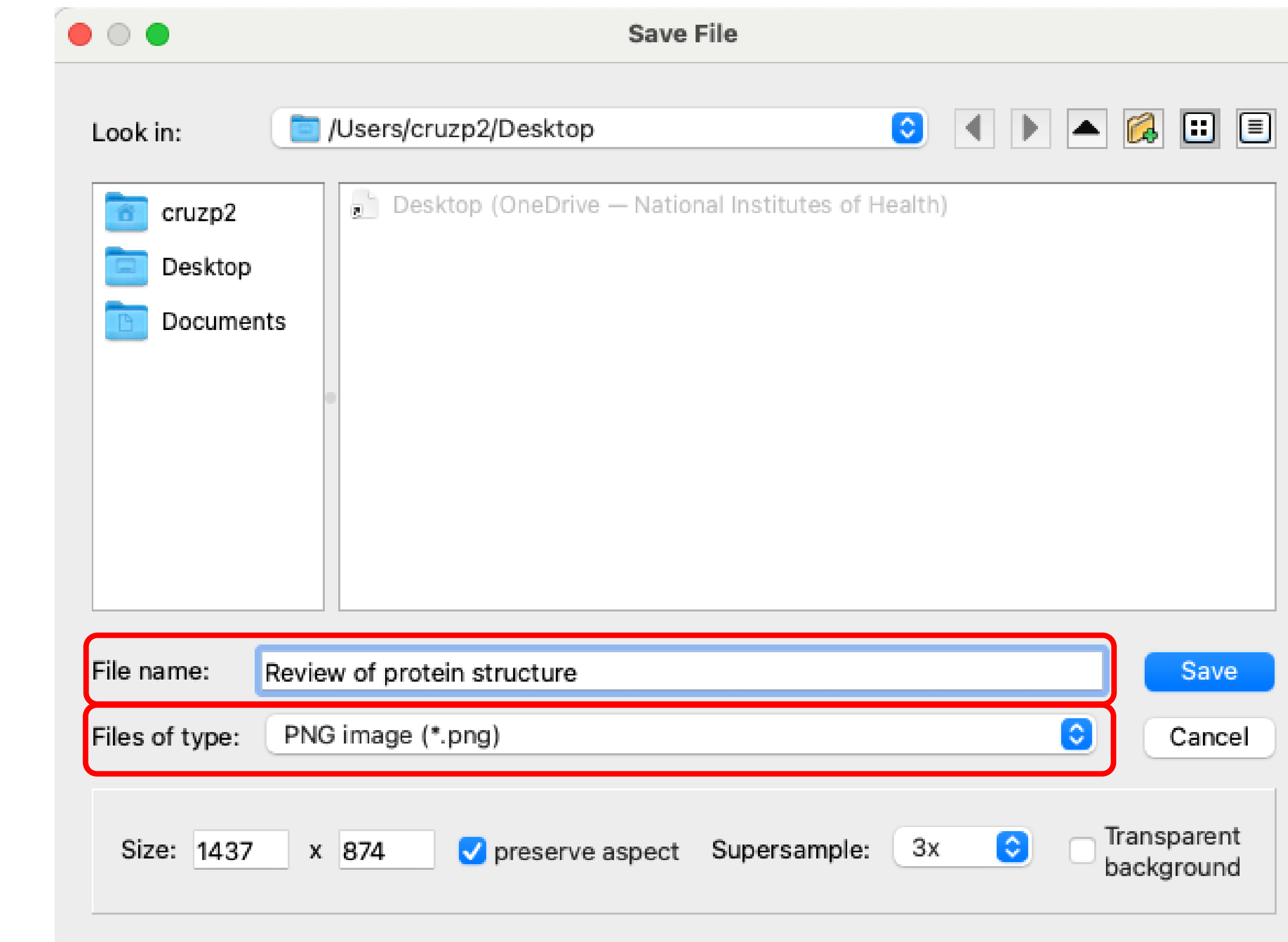


Save as an image file

1. File>>Save
2. In “Files of type:” choose:
PNG image (*.png)

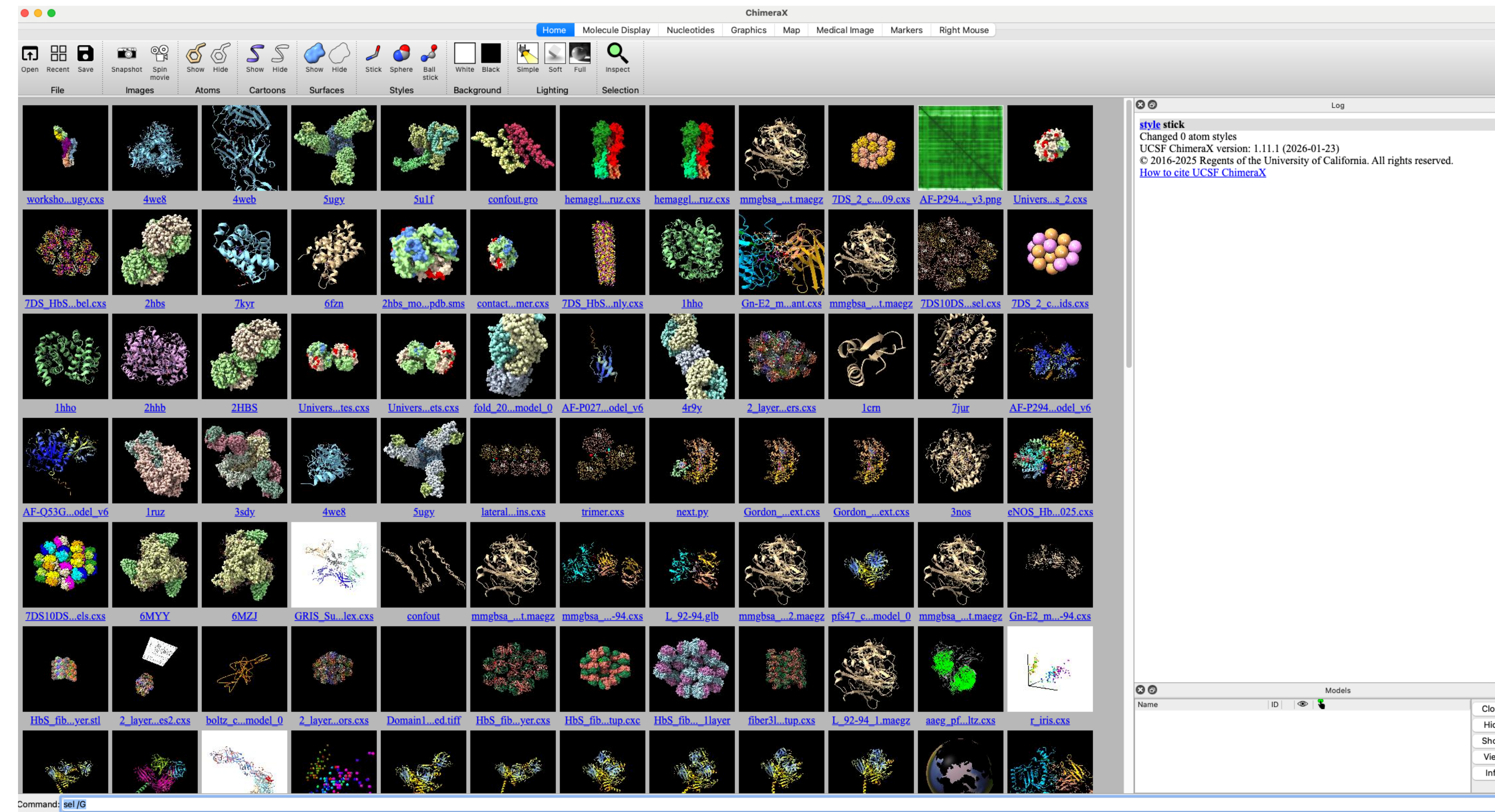
Note that there are additional options; keep the defaults.

3. Enter a file name
 4. Click “Save”.
- Different file types may have different additional options.
5. Quit ChimeraX

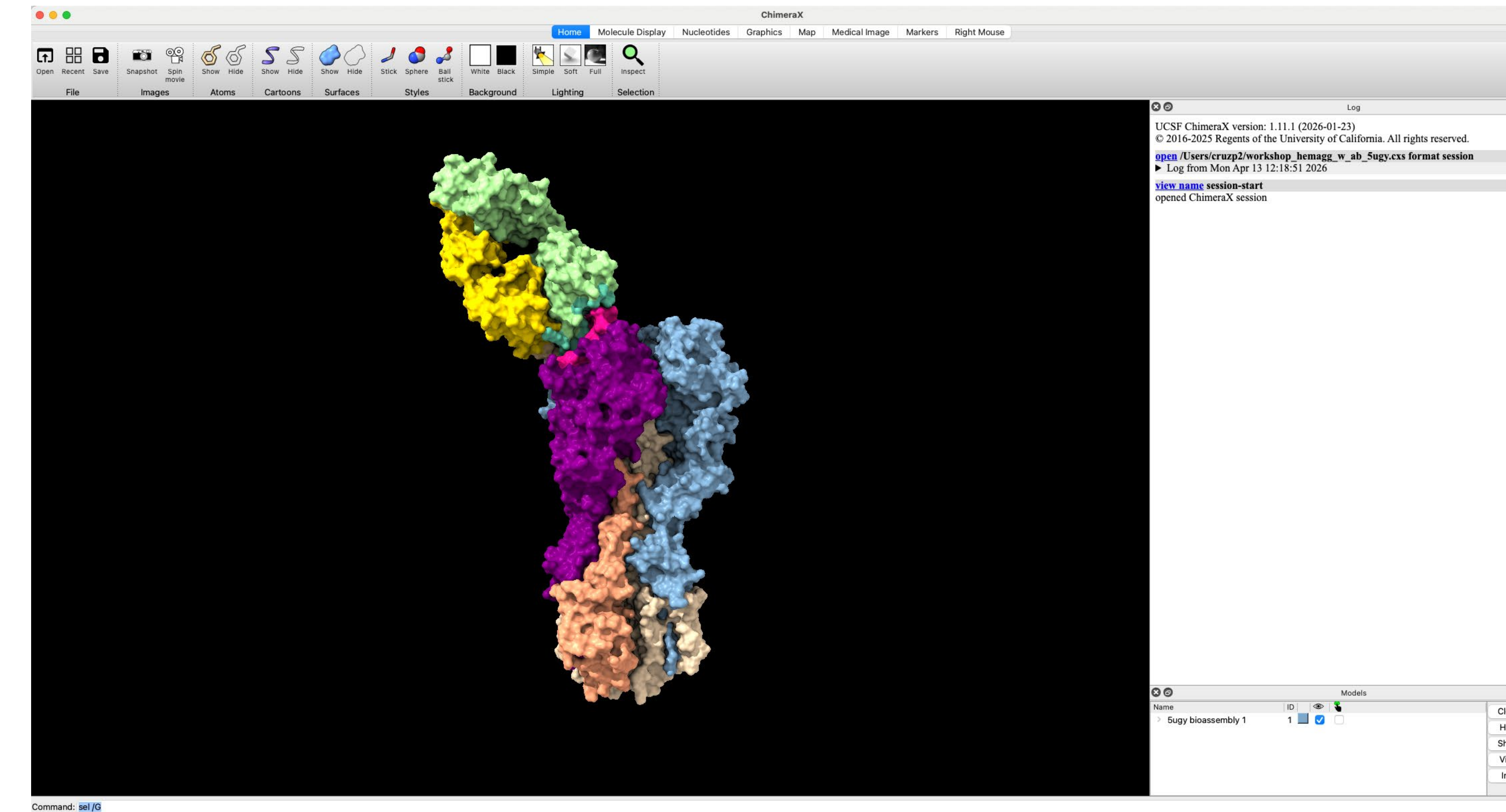


ChimeraX- Exercise 2: Prepare Hemagglutinin VR scene

ChimeraX window at startup



ChimeraX window after opening a session file: .cxs



PDB: Influenza hemagglutinin with antibody PDB entry 5UGY

RCSB PDB- <https://www.rcsb.org>

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RCSB PDB PROTEIN DATA BANK
253,780 Structures from the PDB archive
1,062,058 Computed Structure Models (CSM)
Enter search term(s), Ligand ID or sequence
Include CSM
Advanced Search | Chemical Search | Browse Annotations
Help

PDB-101
PDB
EMDataResource
NAKB
wwPDB Foundation
PDB-IHM
f
X
y
v
in

Structure Summary
Structure
Annotations
Experiment
Sequence
Genome
Ligands
Versions

Biological Assembly 1
Display Files
Download Files
Data API

5UGY | pdb_00005ugy
Influenza hemagglutinin in complex with a neutralizing antibody
PDB DOI: <https://doi.org/10.2210/pdb5UGY/pdb>
Entry: 5UGY supersedes: 3SM5
Classification: VIRAL PROTEIN/IMMUNE SYSTEM
Organism(s): Influenza A virus (A/Solomon Islands/3/2006(H1N1)), Homo sapiens
Expression System: Trichoplusia ni, Homo sapiens
Mutation(s): No
Deposited: 2017-01-10 Released: 2017-01-25
Deposition Author(s): Whittle, J.R.R., Jenni, S., Harrison, S.C.
Experimental Data Snapshot
wwPDB Validation
3D Report
Full Report

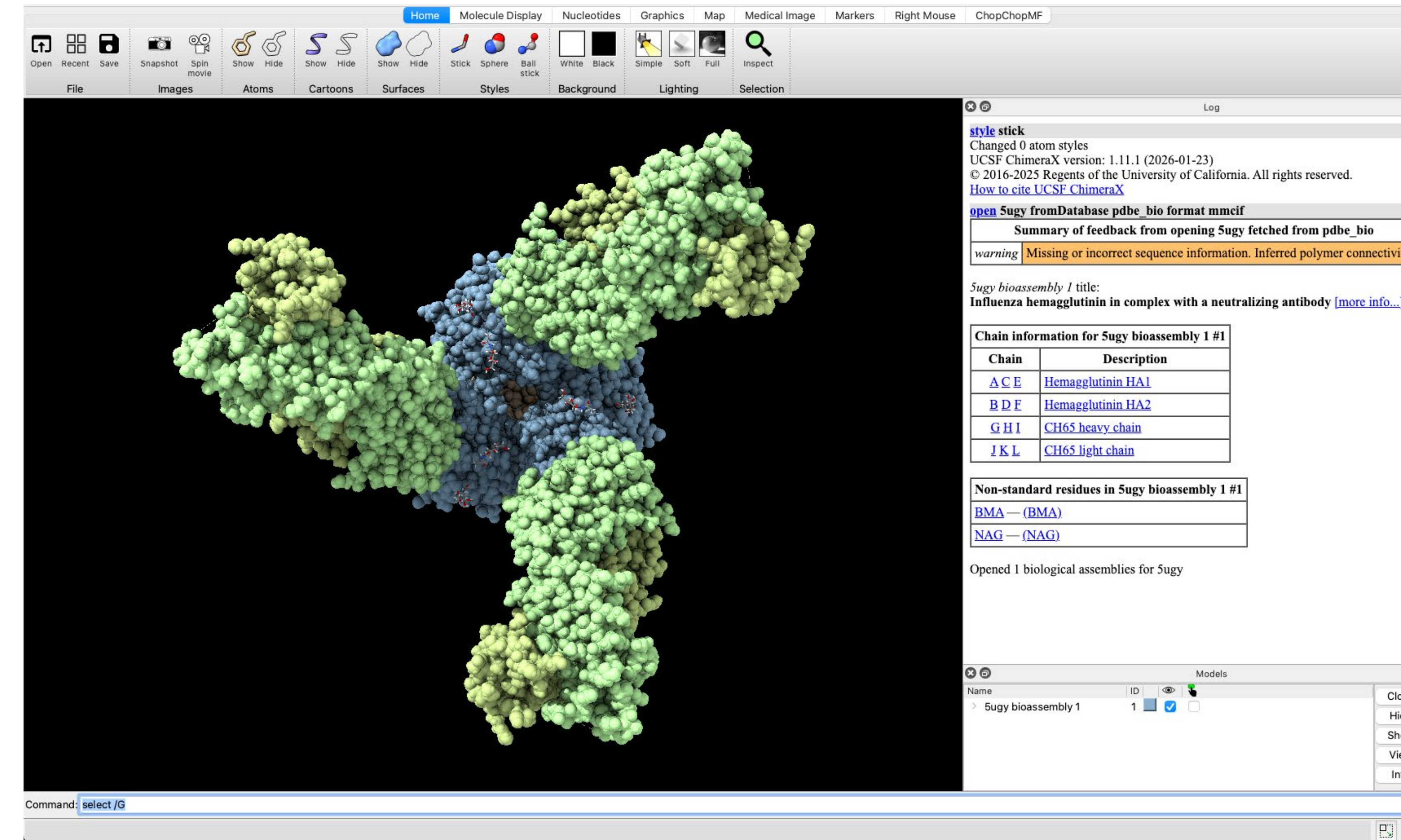
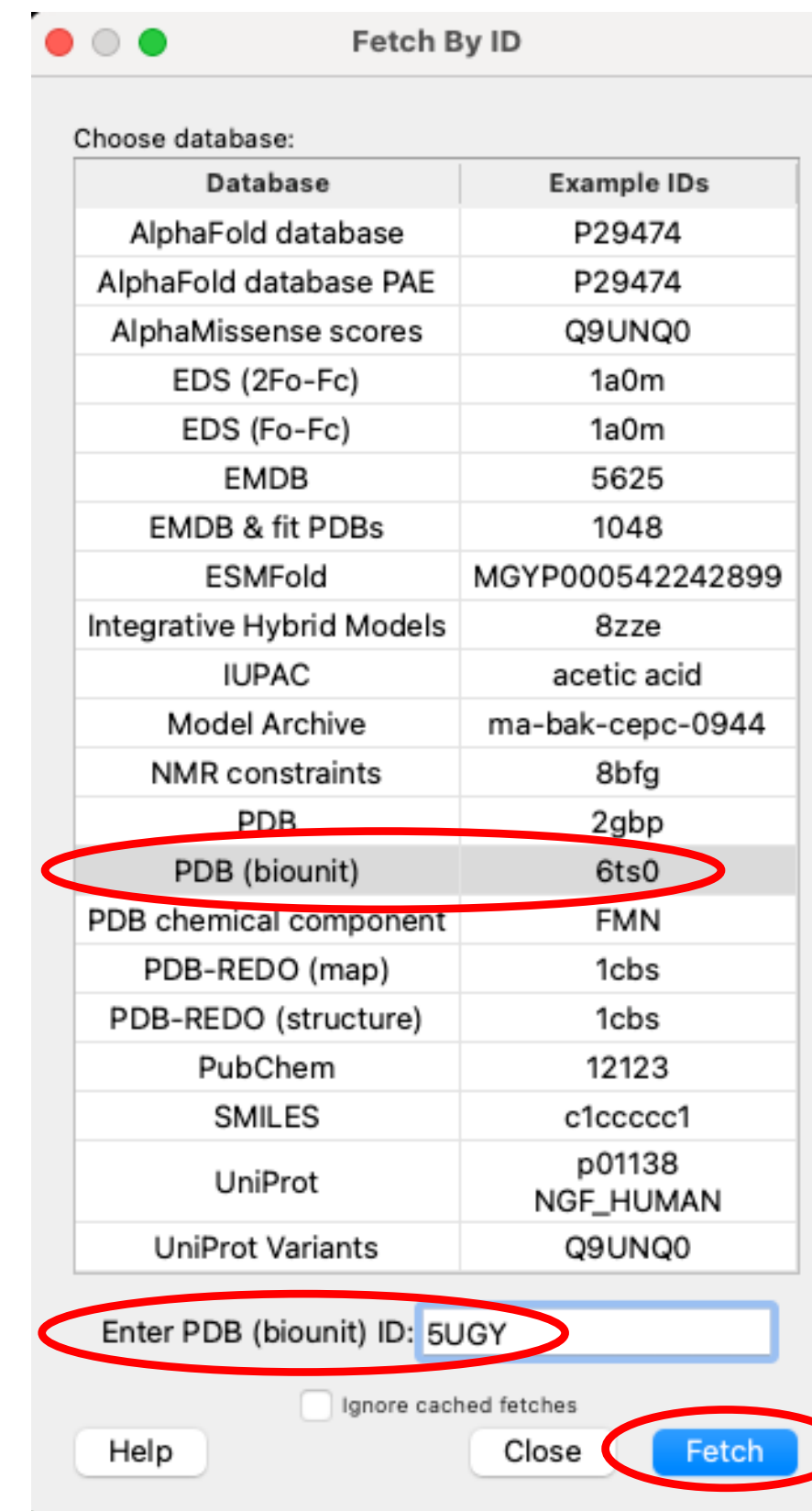


“Fetch” the structure into ChimeraX directly from the PDB

ChimeraX Standard Representation

1. File menu>>Fetch by ID...
2. Choose “PDB (biounit)”
3. Enter 5UGY and click “Fetch”

The structure loads into the ChimeraX graphics window.



Smaller Structures/few chains

- Protein backbone is shown as a ribbons
- Ligands are shown as “sticks”
- Protein sidechains near ligands are shown as sticks
- Water molecules near ligands are shown as a red dots

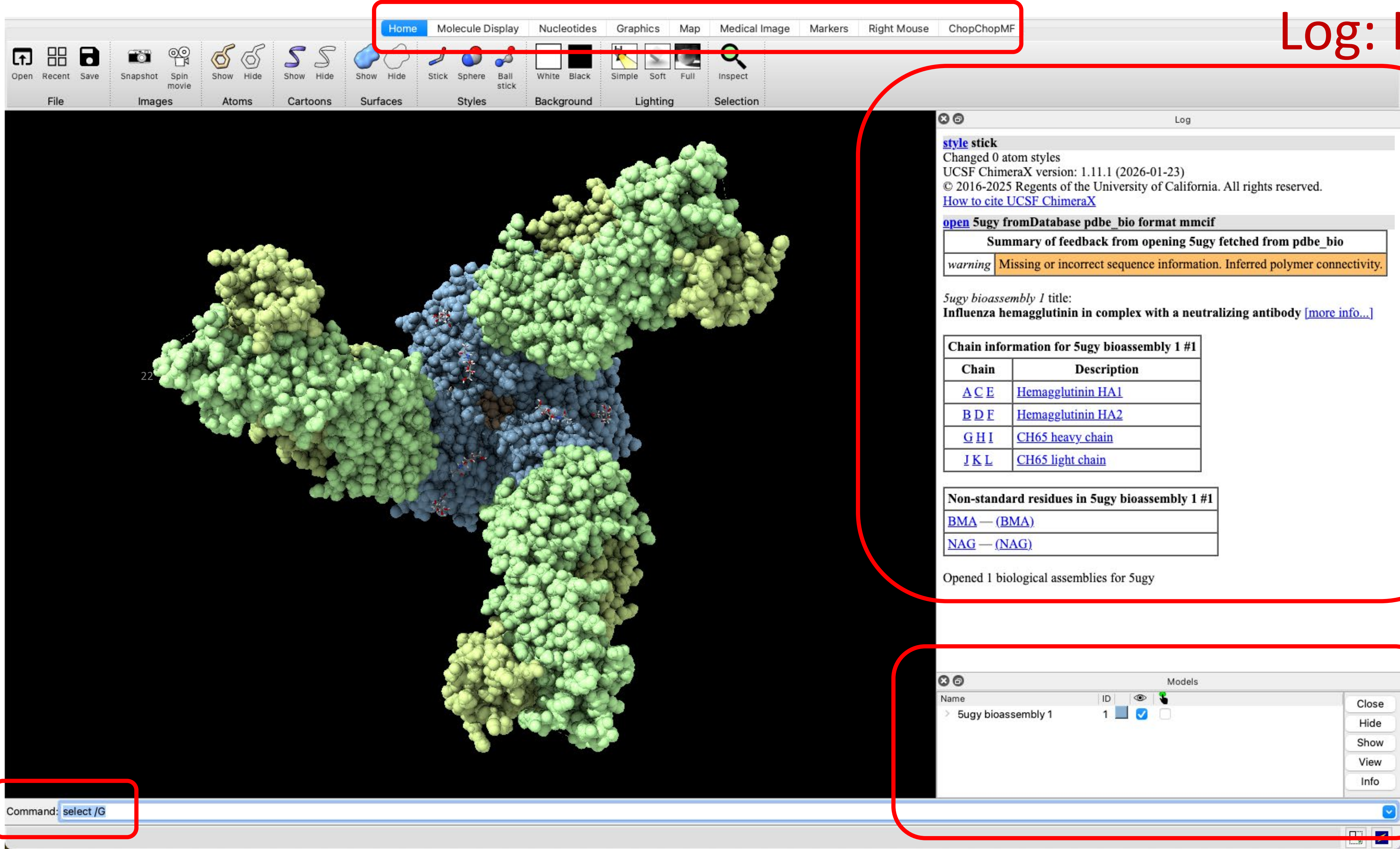
Larger structures/many chains

- Protein atoms shown as spheres
- Ligands are shown as “sticks”
- Water molecules are shown as a red dots

Hovering mouse cursor over part of model gives a popup (tooltip) description

Tabs control toolbar icons below

Log: Includes links derived from PDB



Command Line

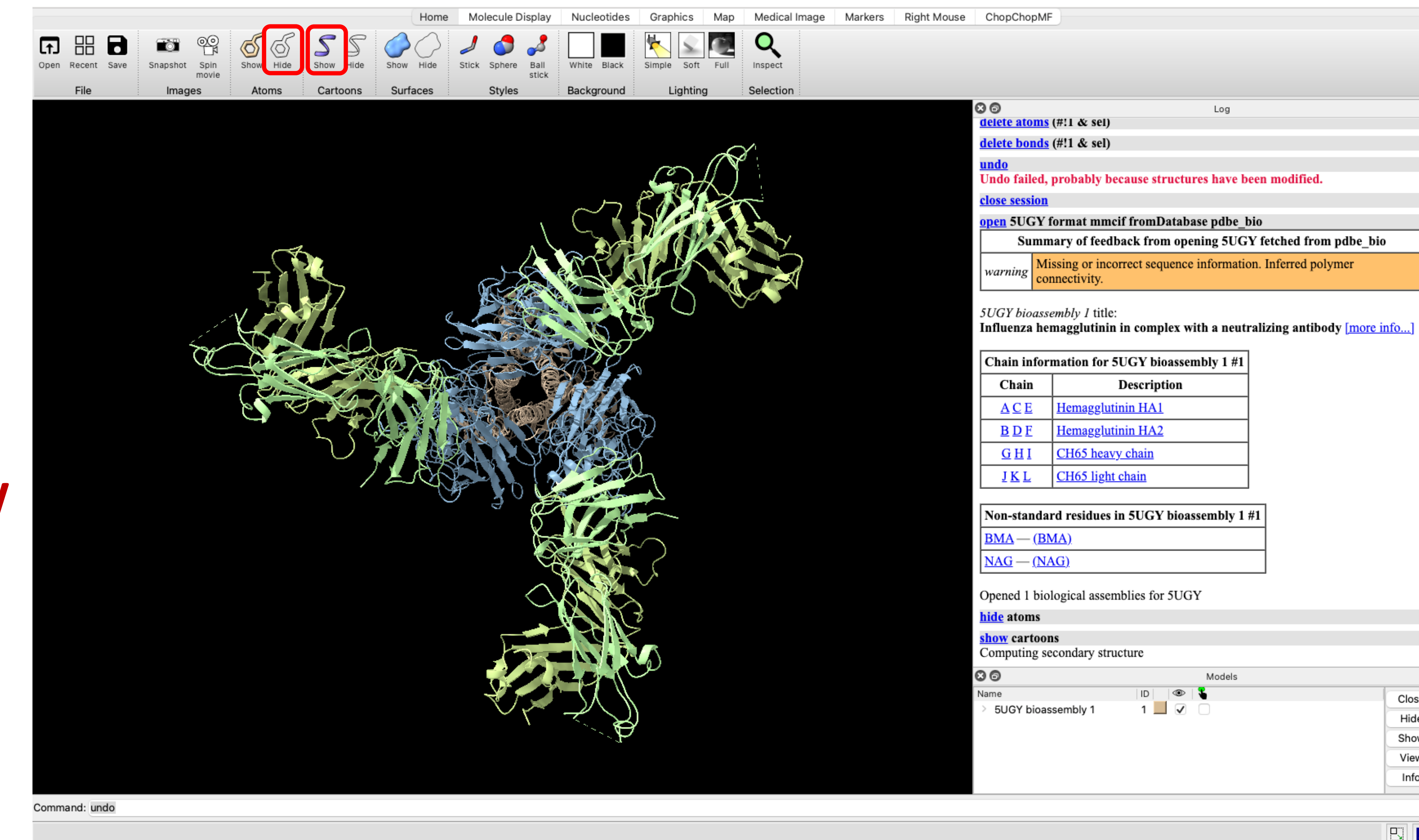
Model Panel

Summary of mouse and trackpad default assignments:

rotate  XY-rotate, except Z-rotate with cursor near edge of window	left mouse button
	trackpad click-drag Mac: also trackpad 2-finger rotation if multitouch gestures enabled
translate 	middle mouse button, right mouse button
	Mac: trackpad + Alt , 3-finger drag if multitouch gestures enabled Windows: trackpad + Ctrl-Alt
+ Shift switches from rotate to translate and <i>vice versa</i> (details...)	
zoom 	mouse scroll wheel
	Mac: trackpad pinch or 4-finger drag if multitouch gestures enabled, otherwise 2-finger drag Windows: trackpad 2-finger drag
select 	left mouse button + Ctrl , + Shift to toggle or add to selection
	trackpad + Ctrl , + Shift to toggle or add to selection

Change representation from atoms to cartoons:

In the toolbar icons click Atoms Hide, then Cartoons Show

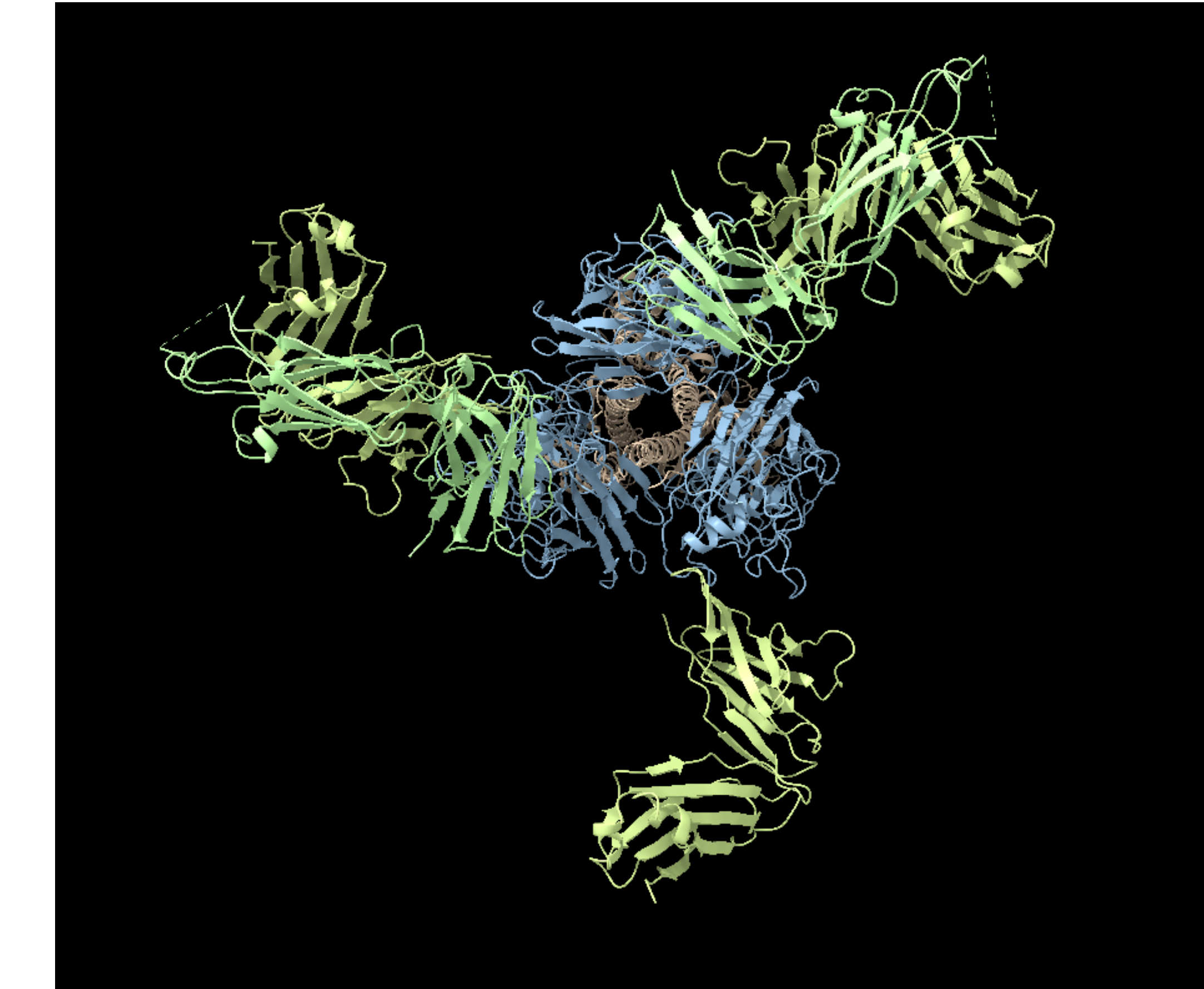
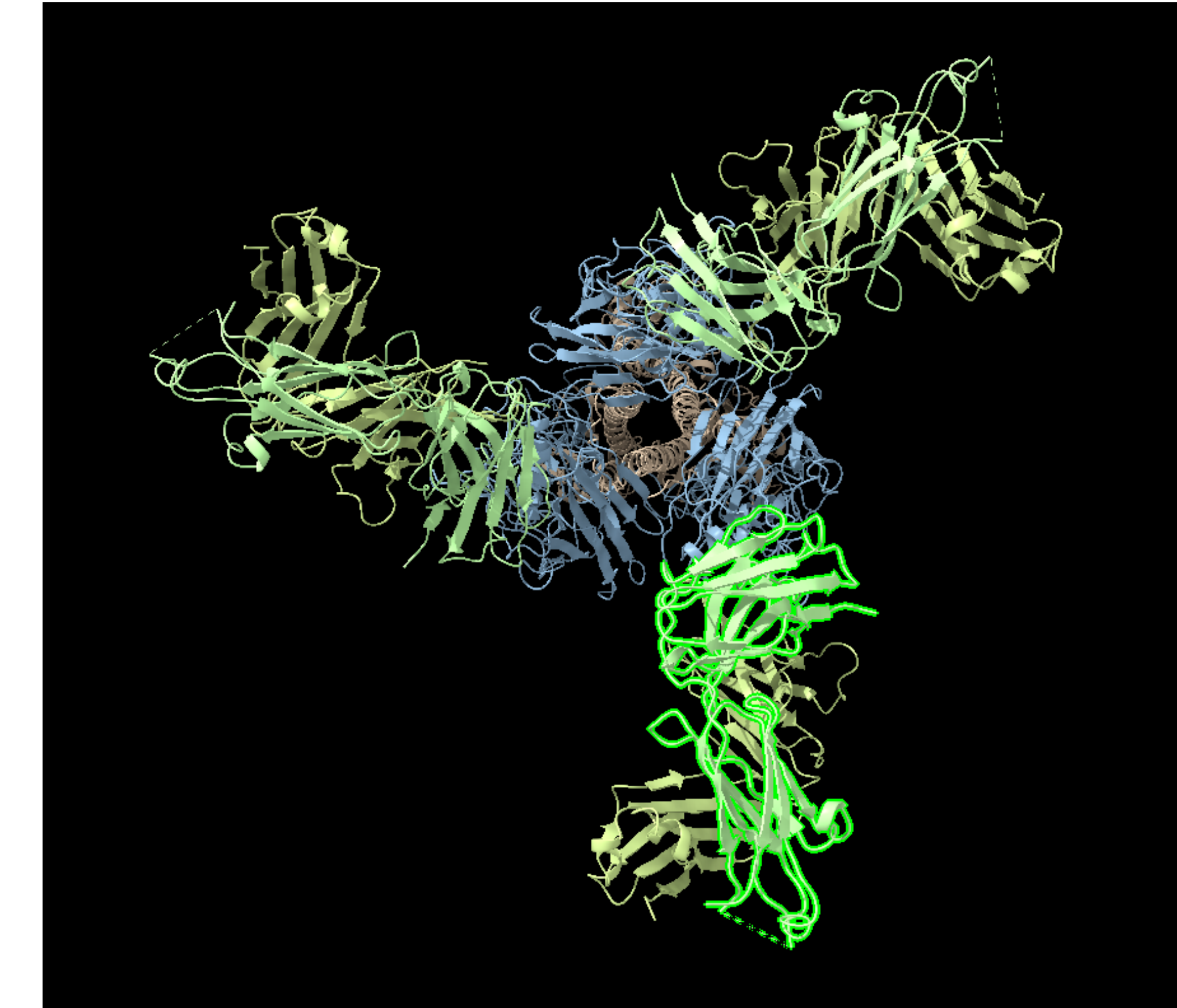


Working with ChimeraX- Paradigm

- Select *then* Actions (on selection)
 - Select can be from the “Select” menu, from the log, on the screen, or from commands
 - Actions can be from the “Actions” menu, or from commands

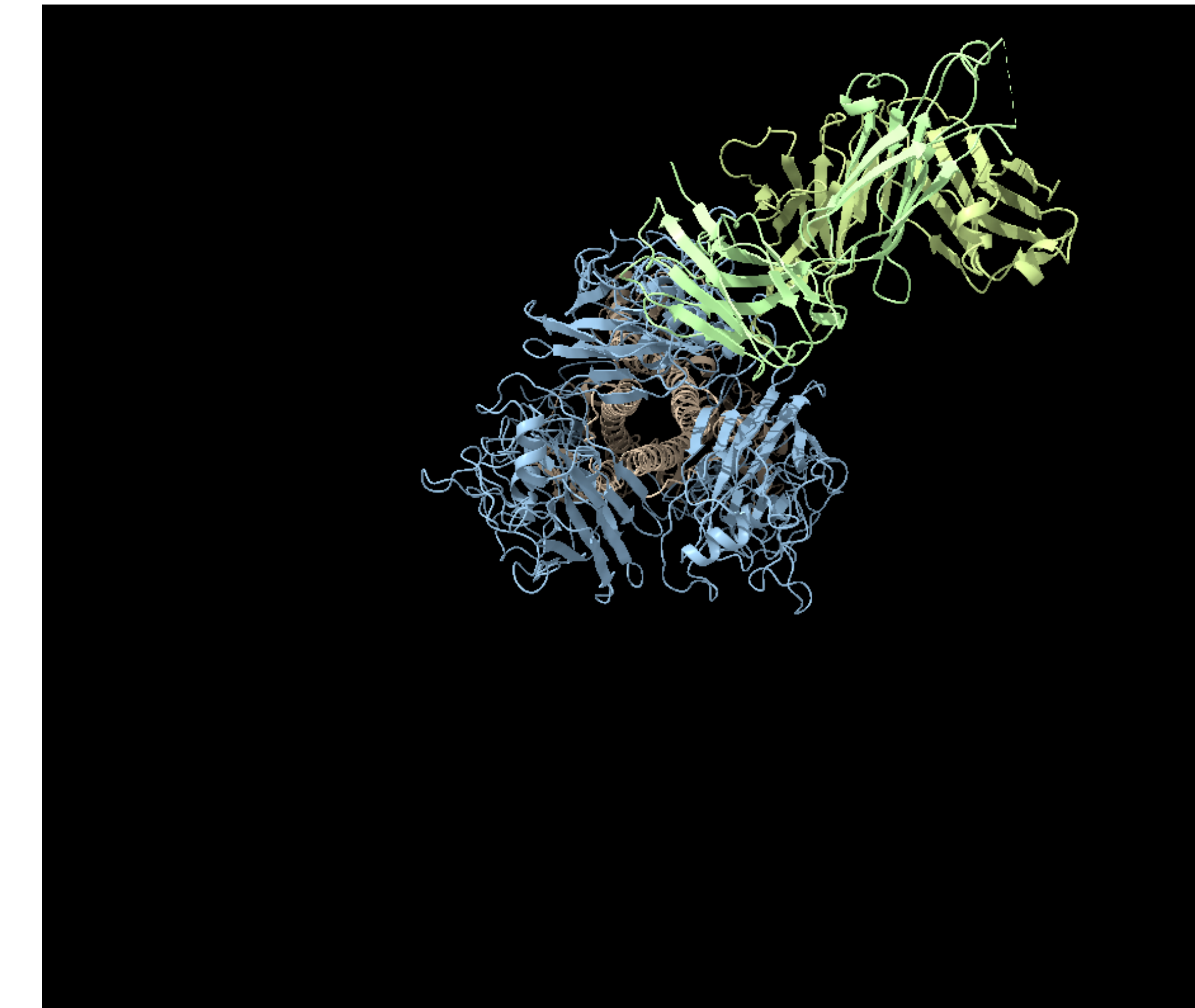
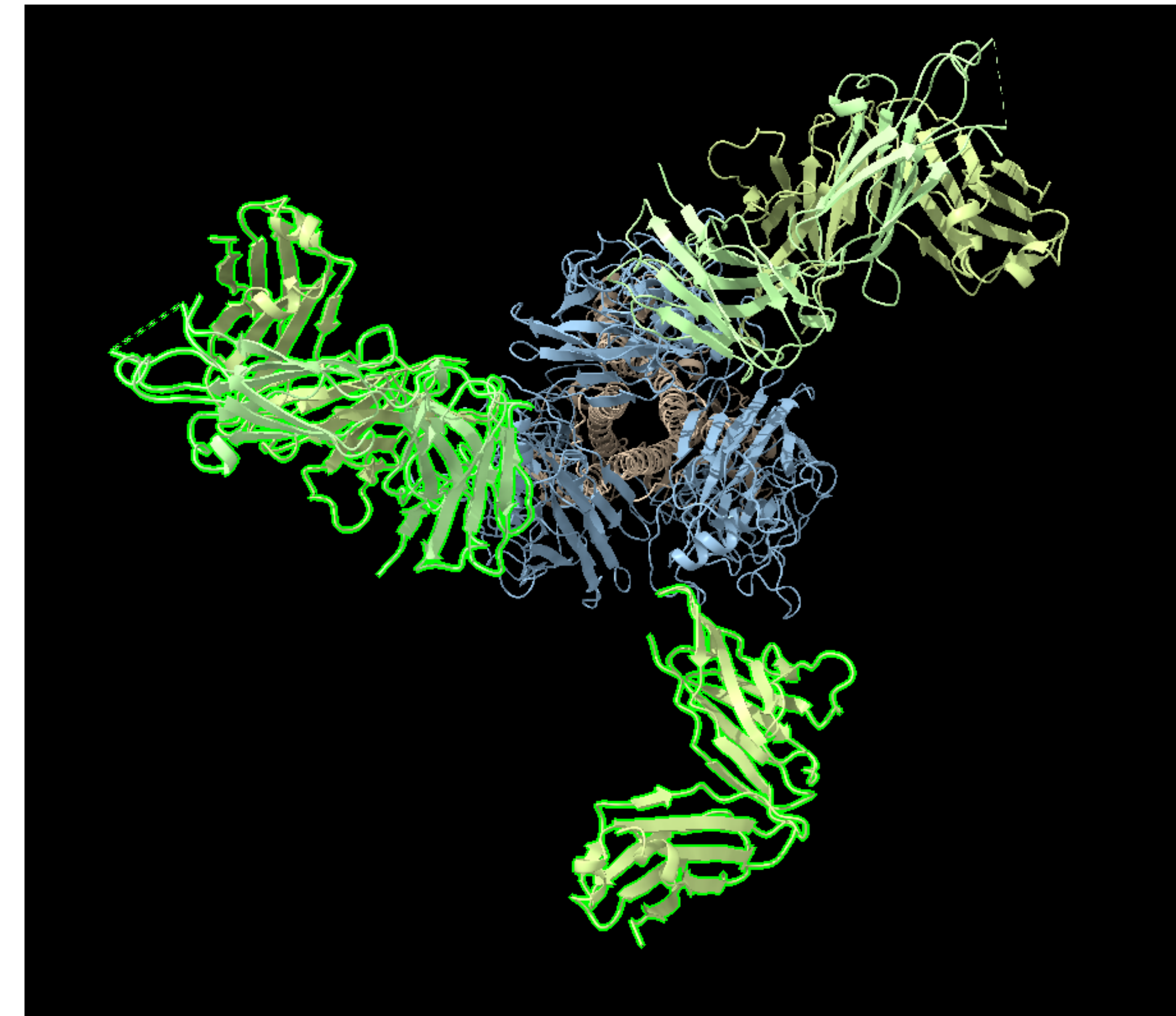
Example: Delete chain “H”

- ²⁴ Step 1- Select
 - From the “Select” menu: Select>>Chains>>CH65 Heavy Chain>>Chain H
 - or
 - Click on the “H” link in the table in the log
 - or
 - Command line type: select #1/H
- Step 2-Actions
 - “Actions” menu: Actions>>Atoms/Bonds>>Delete



Continue deleting chains from 2 of the 3 antibodies

- Step 1- Select
 - Command line type: `sel #1/I,K,L`
- Step 2-Actions
 - Actions>>Atoms/Bonds>>Delete

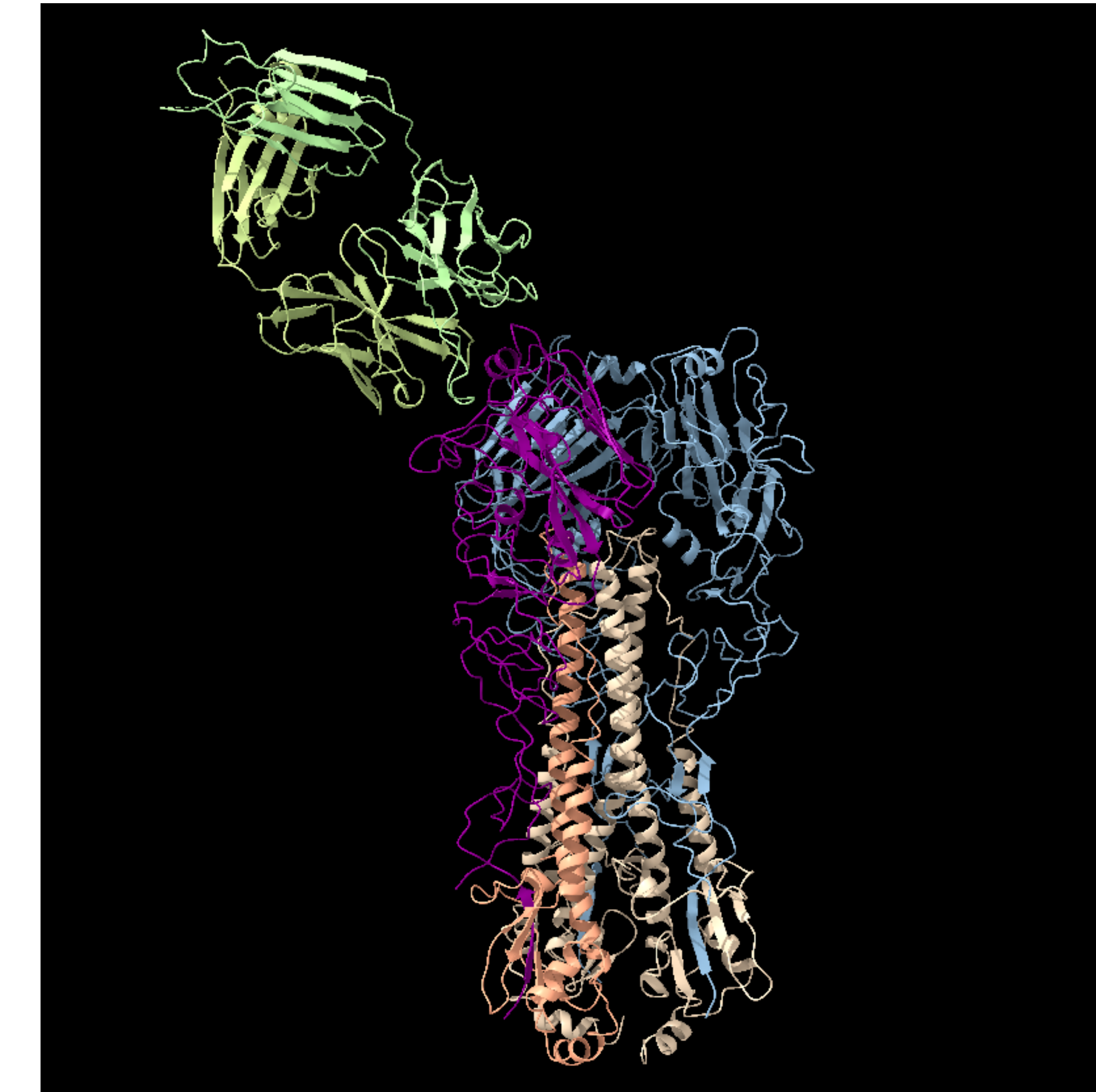
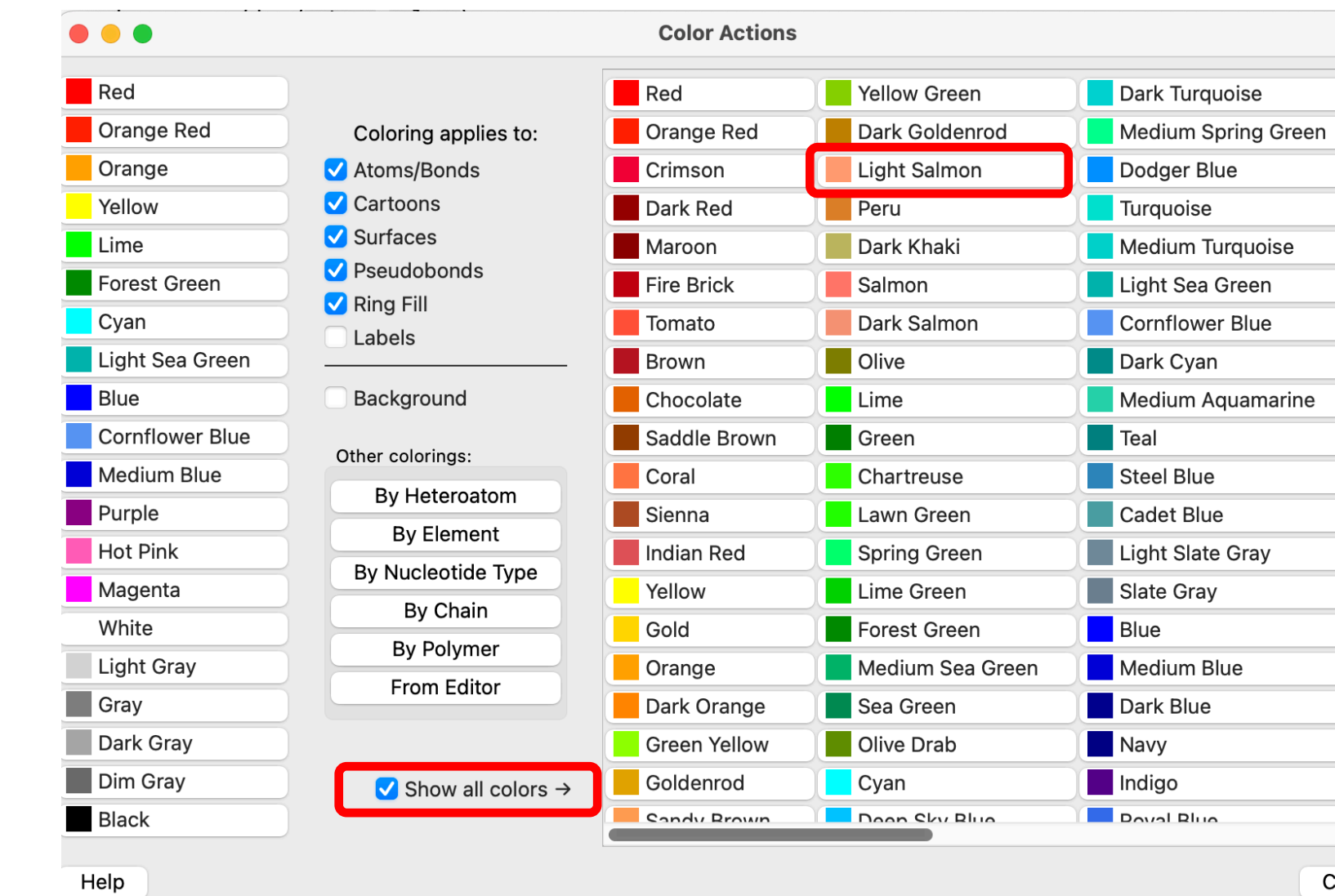


Change colors of one of the hemagglutinin protomers

1. Select>>Chains>>Hemagglutinin HA1>>Chain A
2. Actions>>Color>>Purple
3. Control-click in black area to clear selection



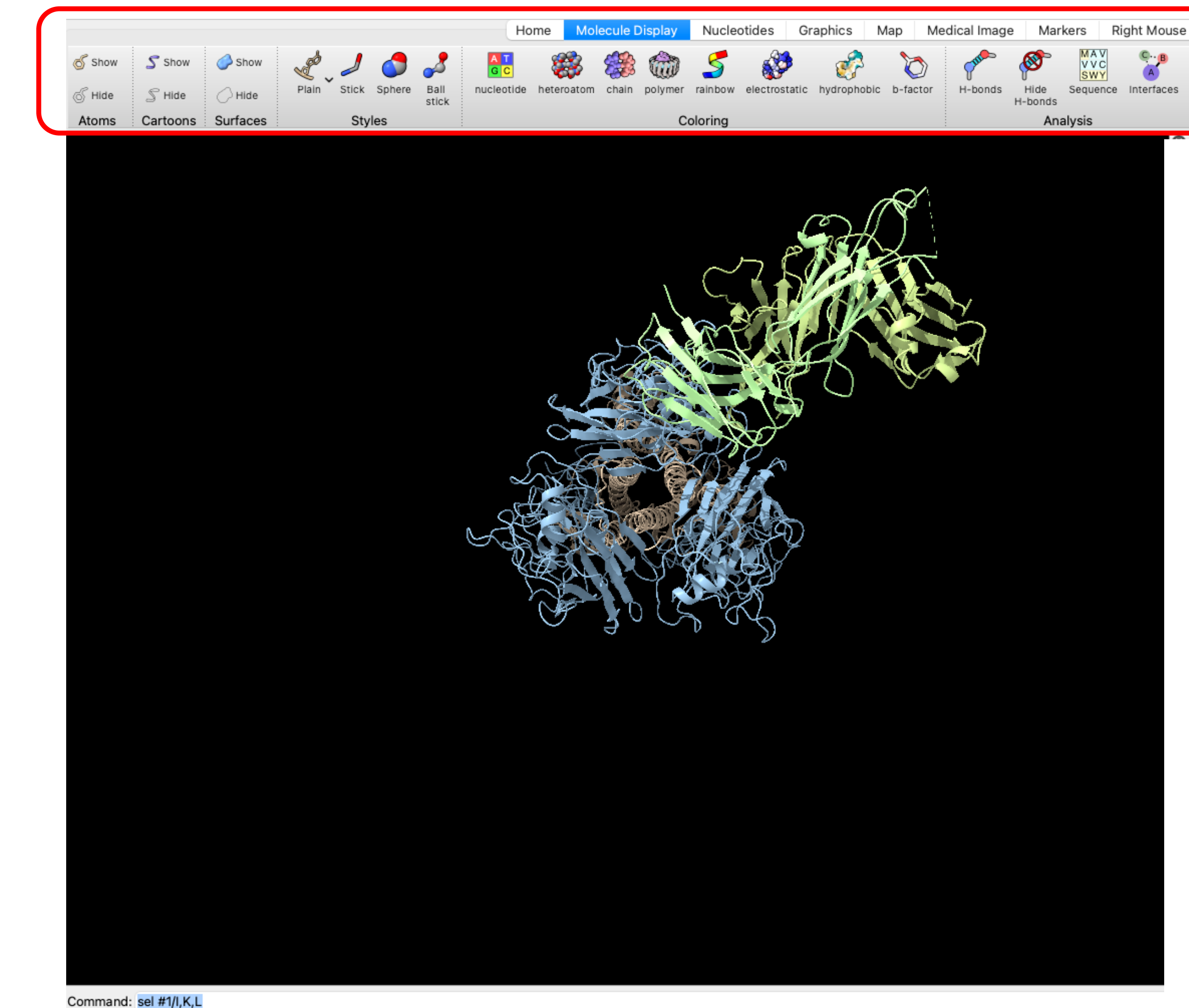
1. Select>>Chains>>Hemagglutinin HA2>>B
2. Actions>>Color>>All Options...
3. Click “Show all colors ->”
4. Click “Light Salmon”
5. Control-click in black area to clear selection



Visualization Options- On Actions menu (Based on current selection)

- Types of molecular visualization
 - Atoms/bonds
 - Stick
 - Ball and Stick
 - Sphere
 - Ribbons
 - **Surfaces**
- Color (Actions menu)
- Labels (Actions menu)

Some Options on Molecule Display Tab

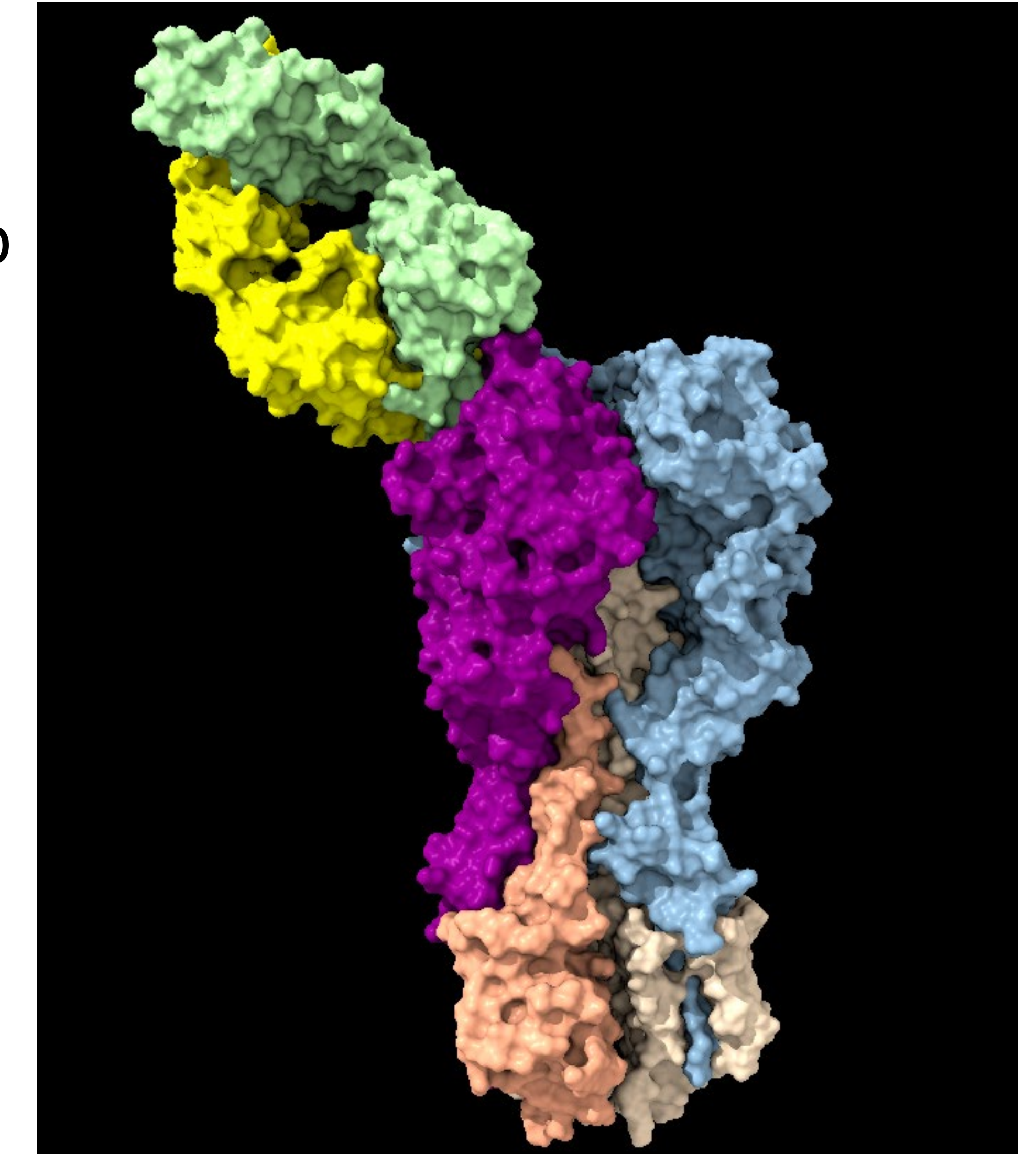


Change colors of the antibody light chain and show surface representation

1. Select>>Chains>>CH65 light chain (chain J)
2. Actions>>Color>>Yellow
3. Control-click in black area to clear selection

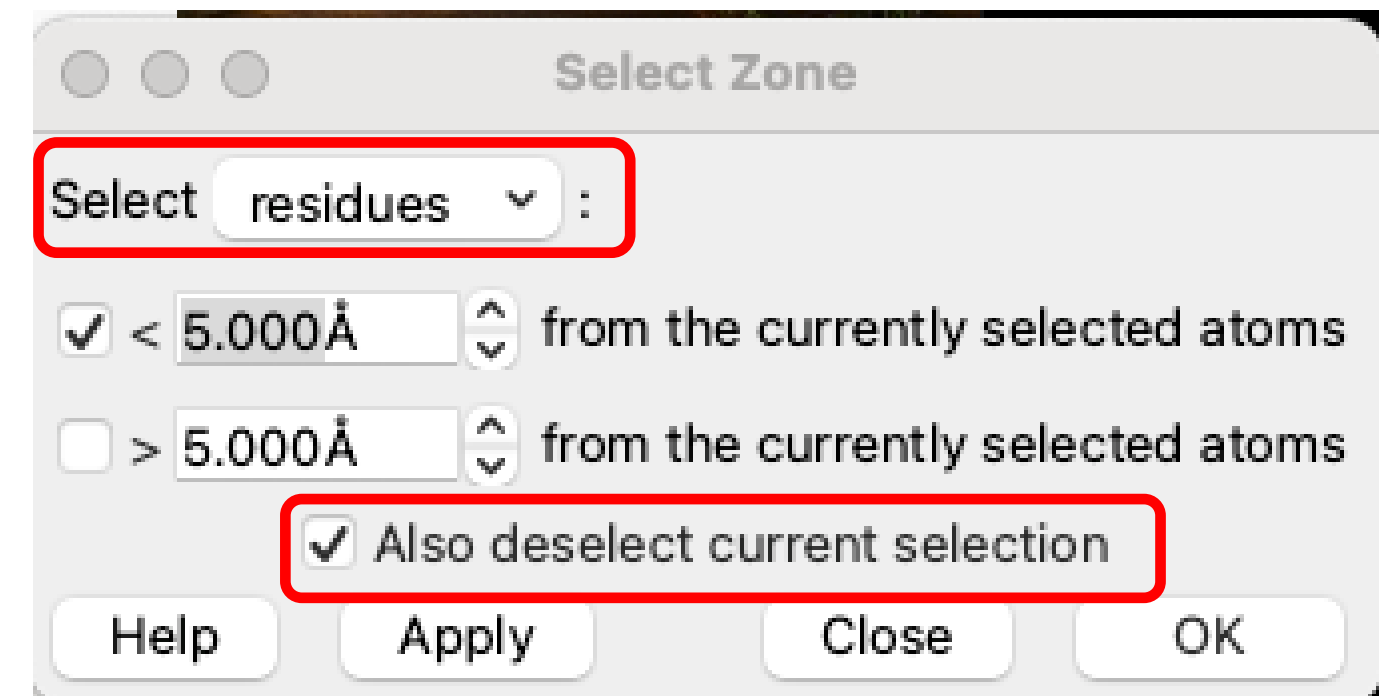


1. Click the “Molecule Display” tab
2. Click “Surfaces Show” icon



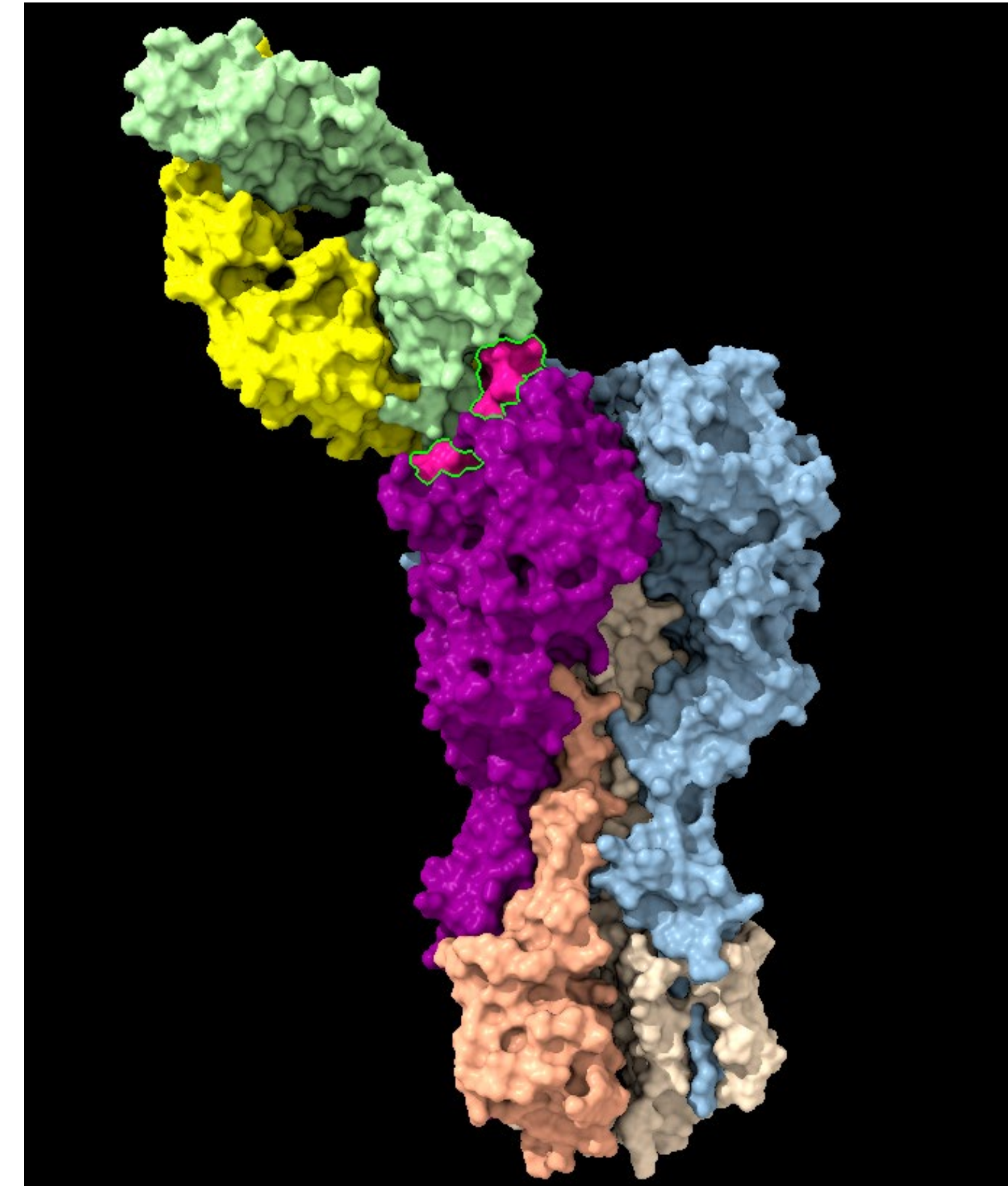
Color the interface between hemagglutinin and antibody heavy chain

1. On the command line type: `sel #1/G`
2. `Select>>Zone...`
3. Change “Select” to “residues” and check “Also deselect...”. Click Apply



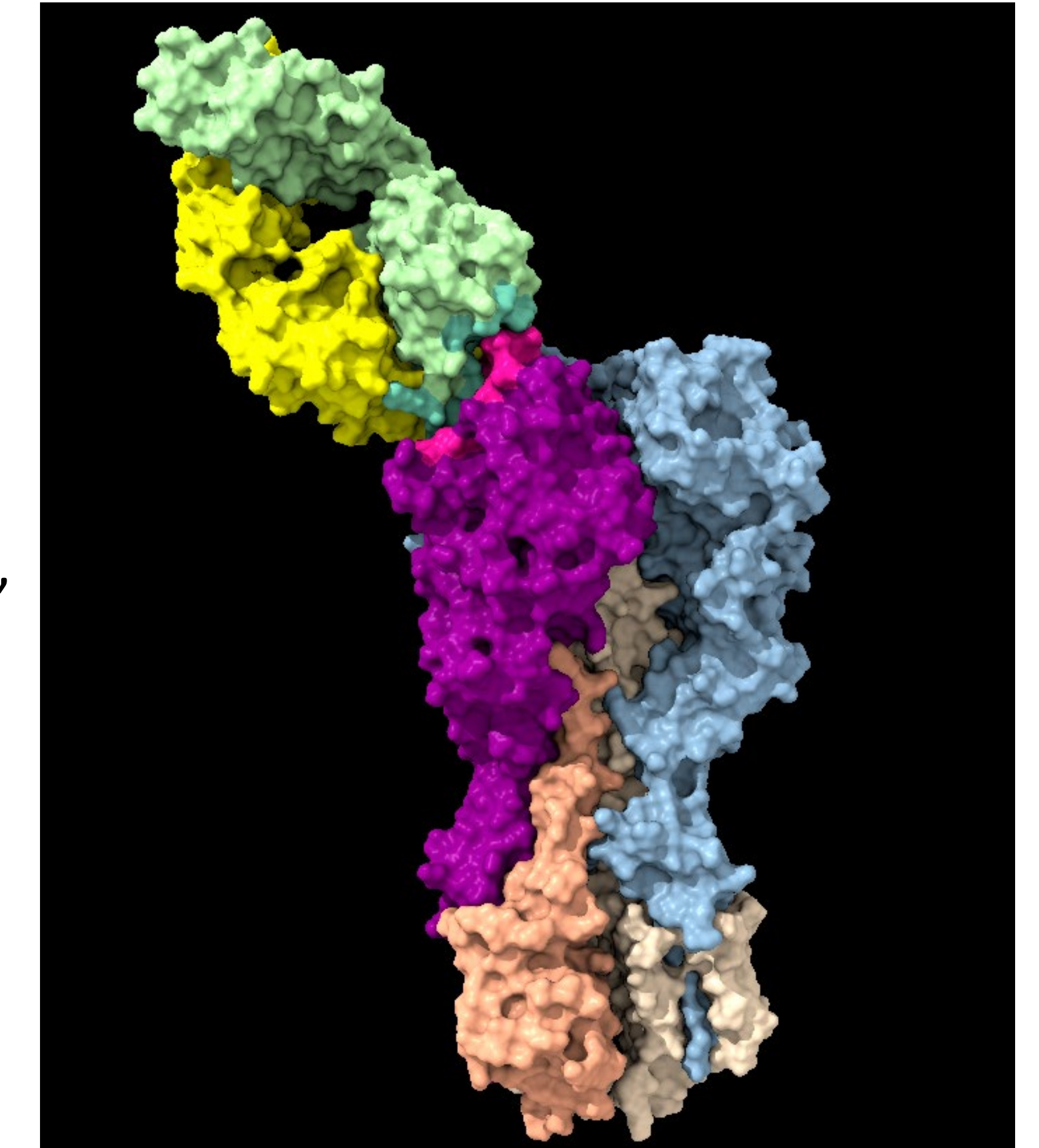
4. `sel sel/A`
This only selects chain A in current selection
Note: Don't change the current selection

5. Color Actions Dialog box: click “Deep Pink”



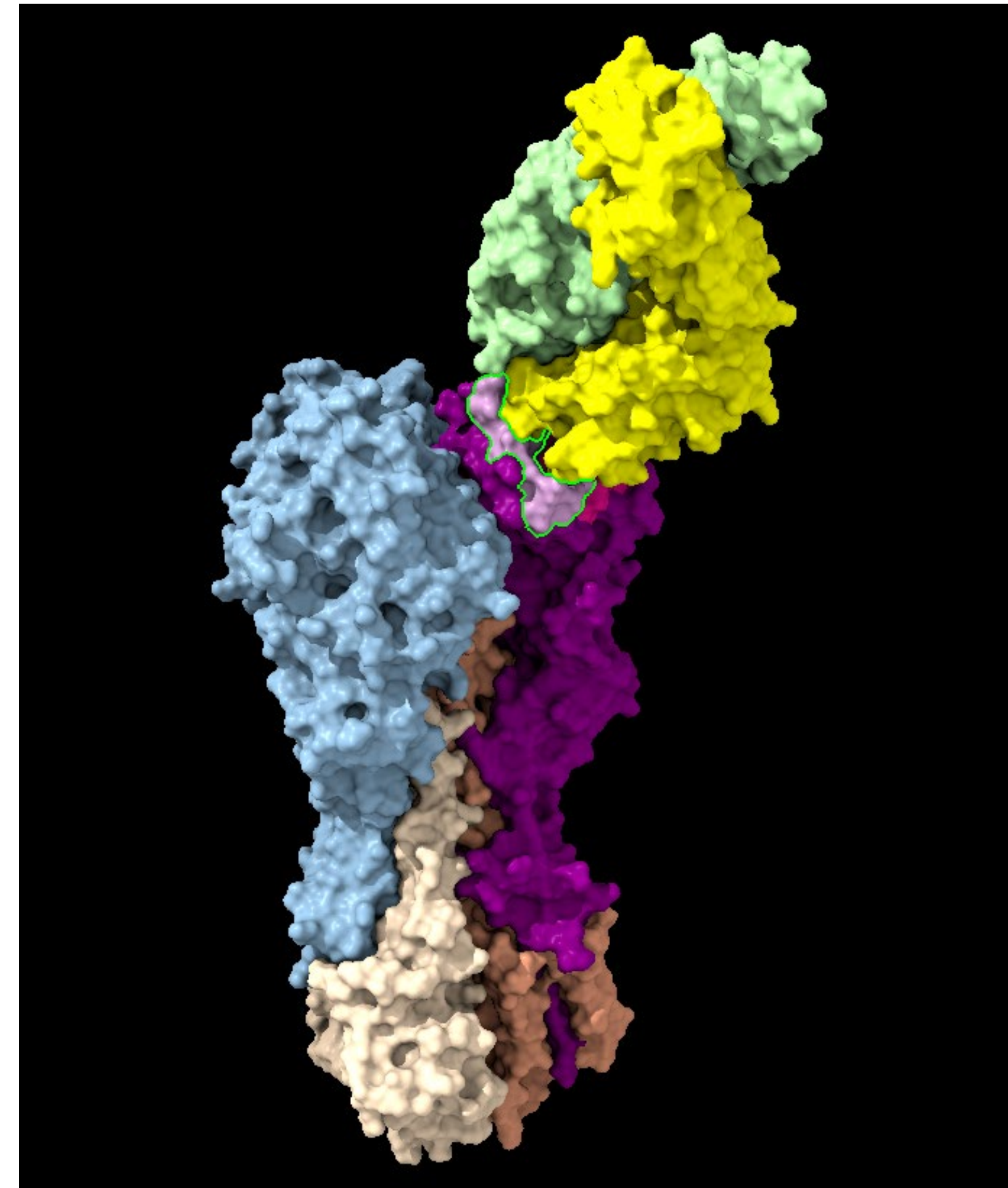
Now color the antibody side of the interface:

1. `Select>>Zone...`
2. Click Apply
3. `sel sel&/G`
This only selects chain G in current selection
4. Color Actions Dialog box: click “Medium Aquamarine”
5. Clear selection



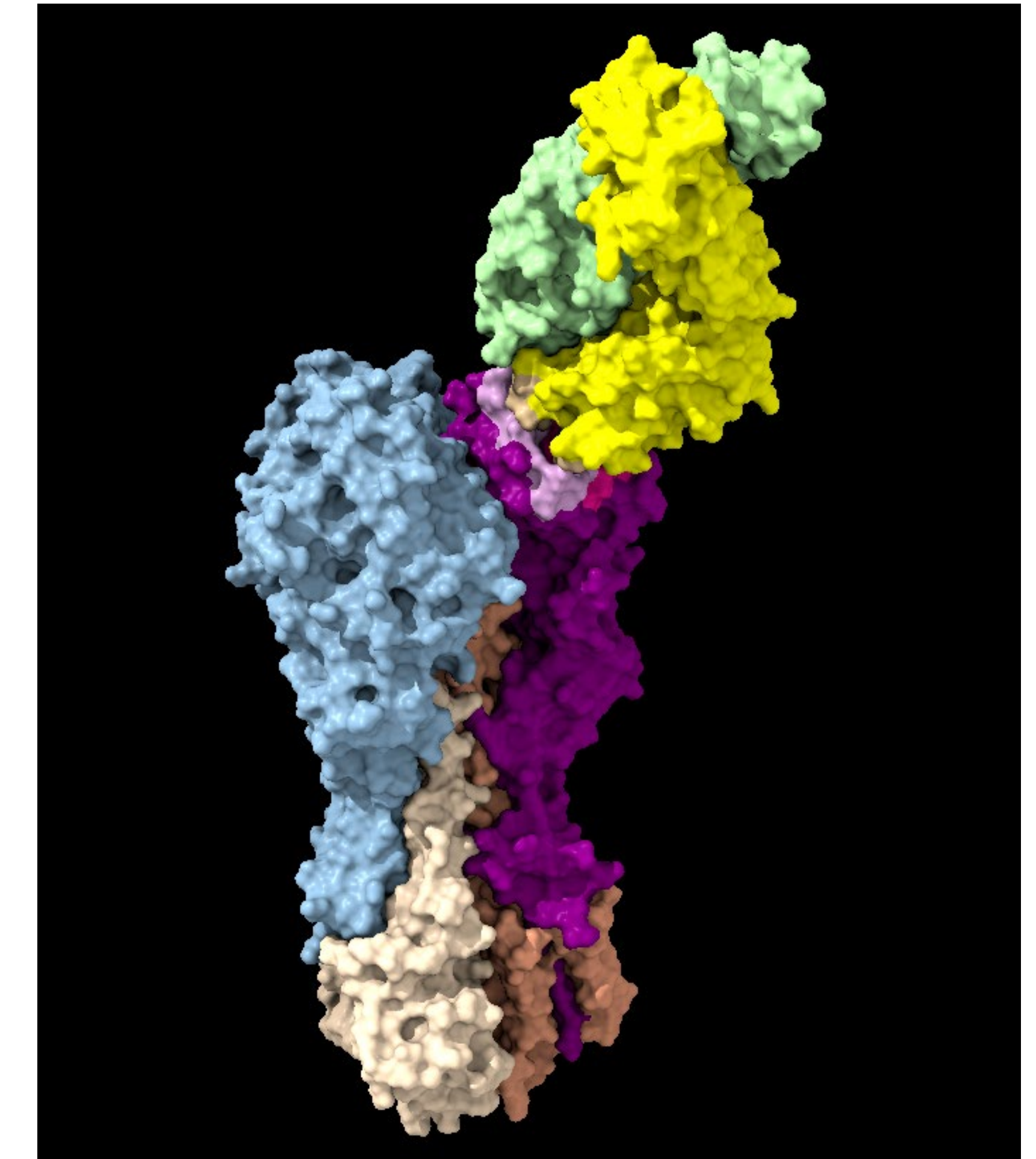
Color the interface between hemagglutinin and the antibody light chain

1. sel #1/J
2. Select>>Zone...
3. Click "Apply" in the dialog box
4. sel sel/A
5. Color Actions Dialog box: click "Plum"



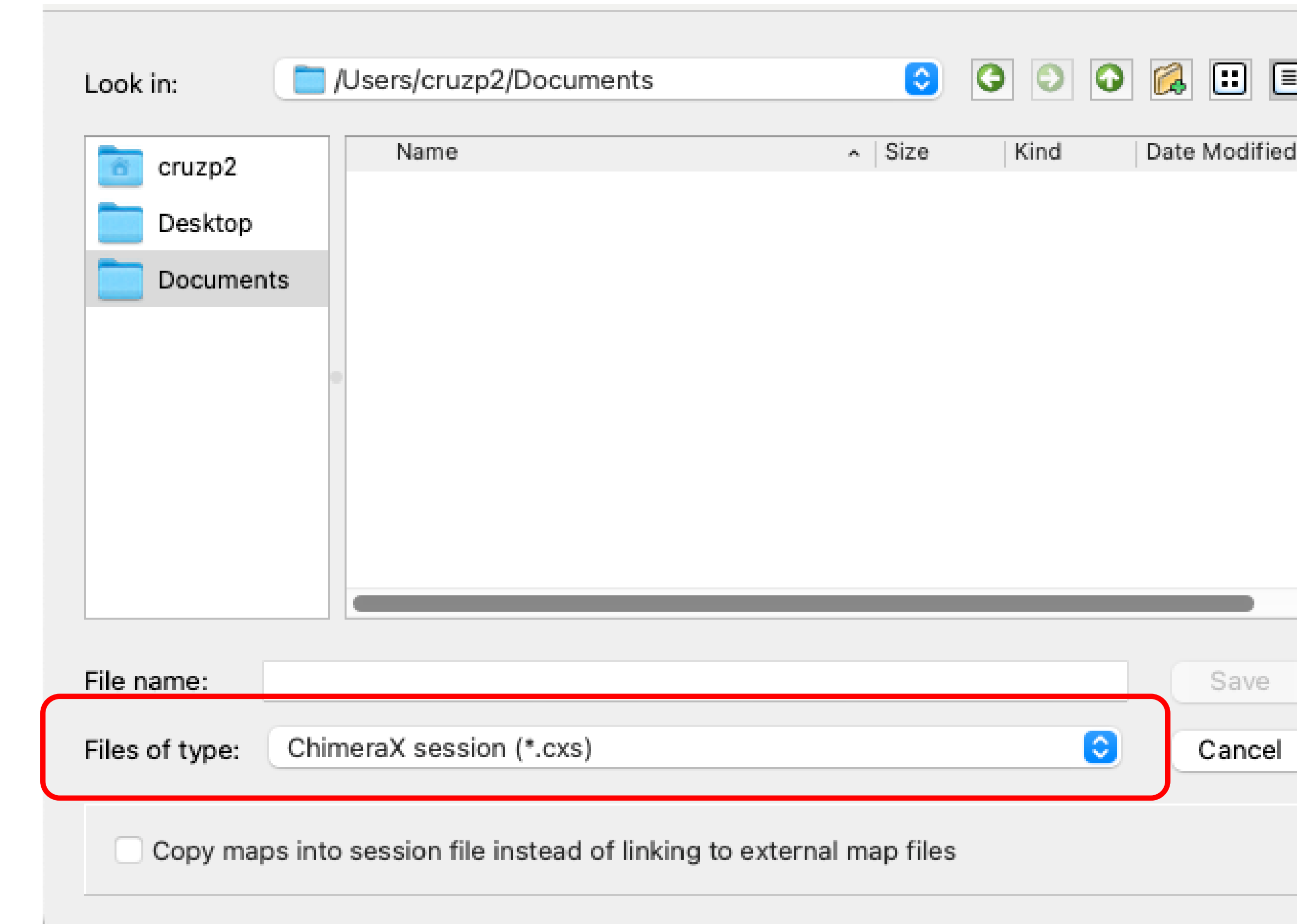
Now color the antibody side of the interface

1. Select>>Zone...
2. Click Apply
3. sel sel/J
4. Color Actions Dialog box: click "Burly Wood"
5. Control-click in the background to deselect everything.



Save current layout as a ChimeraX session file

1. File>>Save...
2. Make sure “Files of type:” is set to ChimeraX session (*.cxs)
3. Enter a file name and click “Save”.



Third Hands-on Exercise: Plasmodium Falciparum Dihydrofolate Reductase: PDB entry 4DPD

Target of antimalarial drugs, with compromised efficacy due to resistance arising from mutations on the enzyme.

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RCSB PDB PROTEIN DATA BANK 181535 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Enter search terms or PDB ID(s). Advanced Search | Browse Annotations Help

CEBB PDB-101 WORLDWIDE PDB PROTEIN DATA BANK EMDDataResource Unified Data Resource for 3DEM ndb NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation Celebrating 50 YEARS OF Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Ligands Versions

Biological Assembly 1

4DPD

WILD TYPE PLASMODIUM FALCIPARUM DIHYDROFOLATE REDUCTASE-THYMIDYLATE SYNTHASE (PfDHFR-TS), DHF COMPLEX, NADP+, dUMP

DOI: 10.2210/pdb4DPD/pdb

Classification: **OXIDOREDUCTASE, TRANSFERASE**

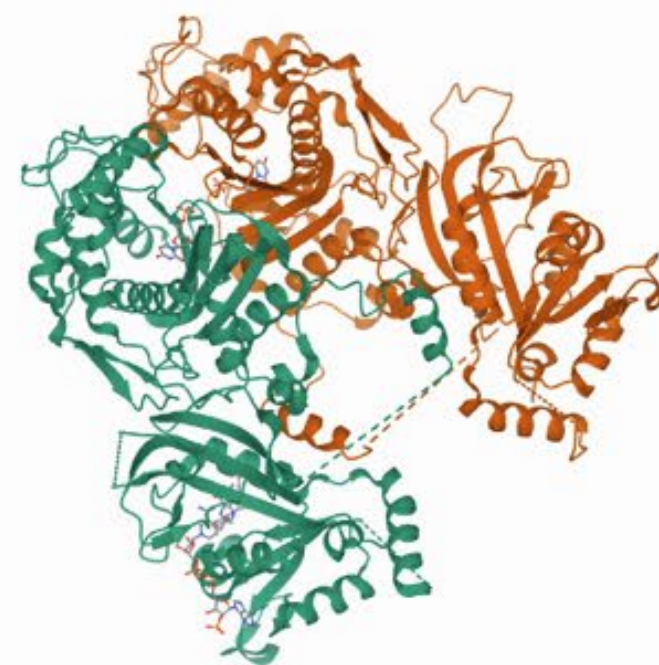
Organism(s): *Plasmodium falciparum*

Expression System: *Escherichia coli*

Mutation(s): No

Deposited: 2012-02-13 Released: 2012-11-14

Deposition Author(s): Yuthavong, Y., Vilaivan, T., Kamchonwongpaisan, S., Charman, S.A., Malaria, B.N., White, K.L., Vignat, B., Reed, E., Chitambar, B., Tjundhara, B.



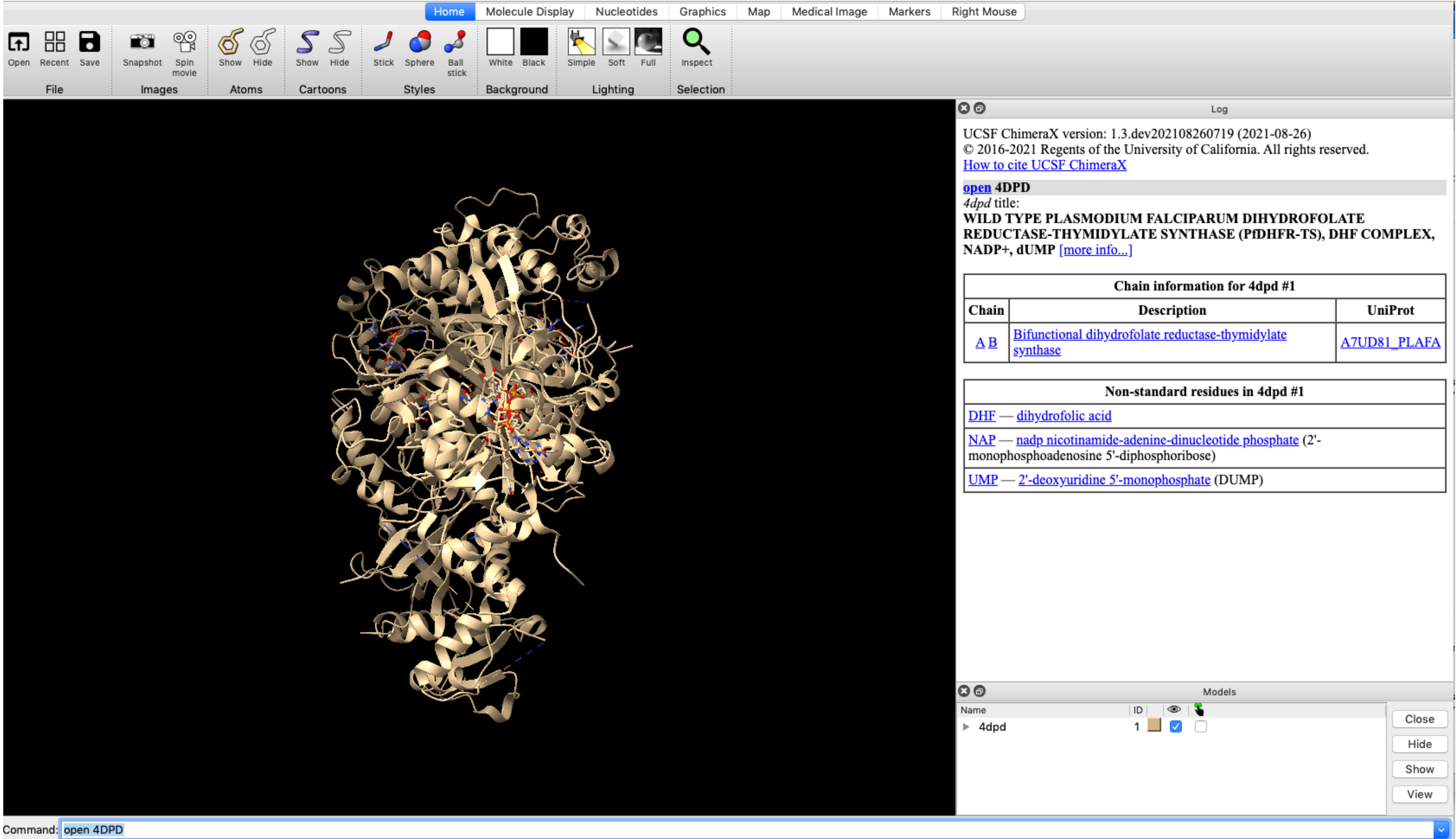
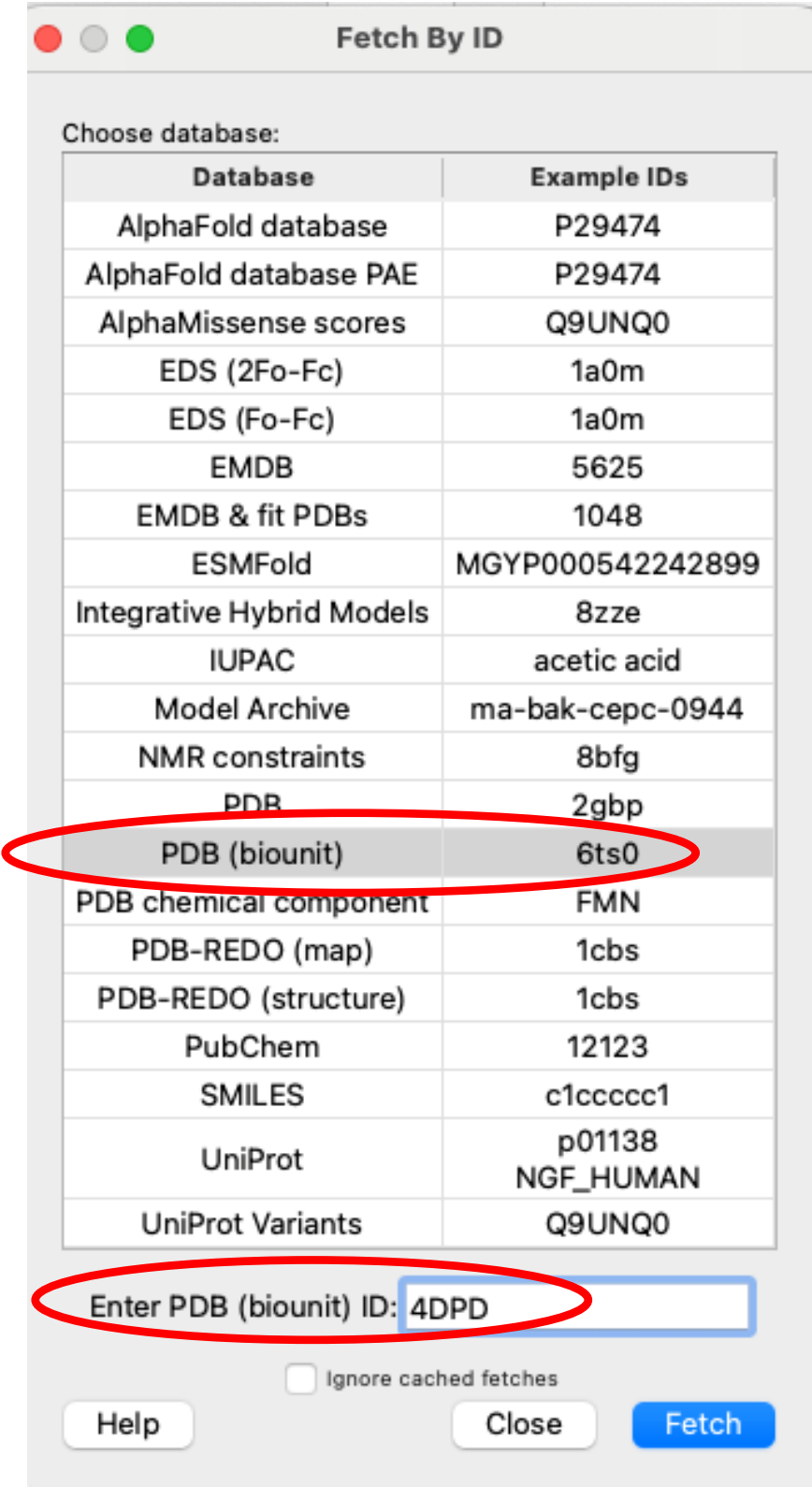
Load the structure into ChimeraX

1. File menu>>Fetch by ID...

2. Choose “PDB (biounit)”

3. Enter 4DPD and click “Fetch”

The structure loads into the ChimeraX graphics window.



Delete Chain B

1. Select Chain B

- From the “Select” menu: Select>>Chains>>Bifunctional ...>>Chain B

or

- Click on the “B” link in the table in the log

or³⁴

- Command line: select #1/B

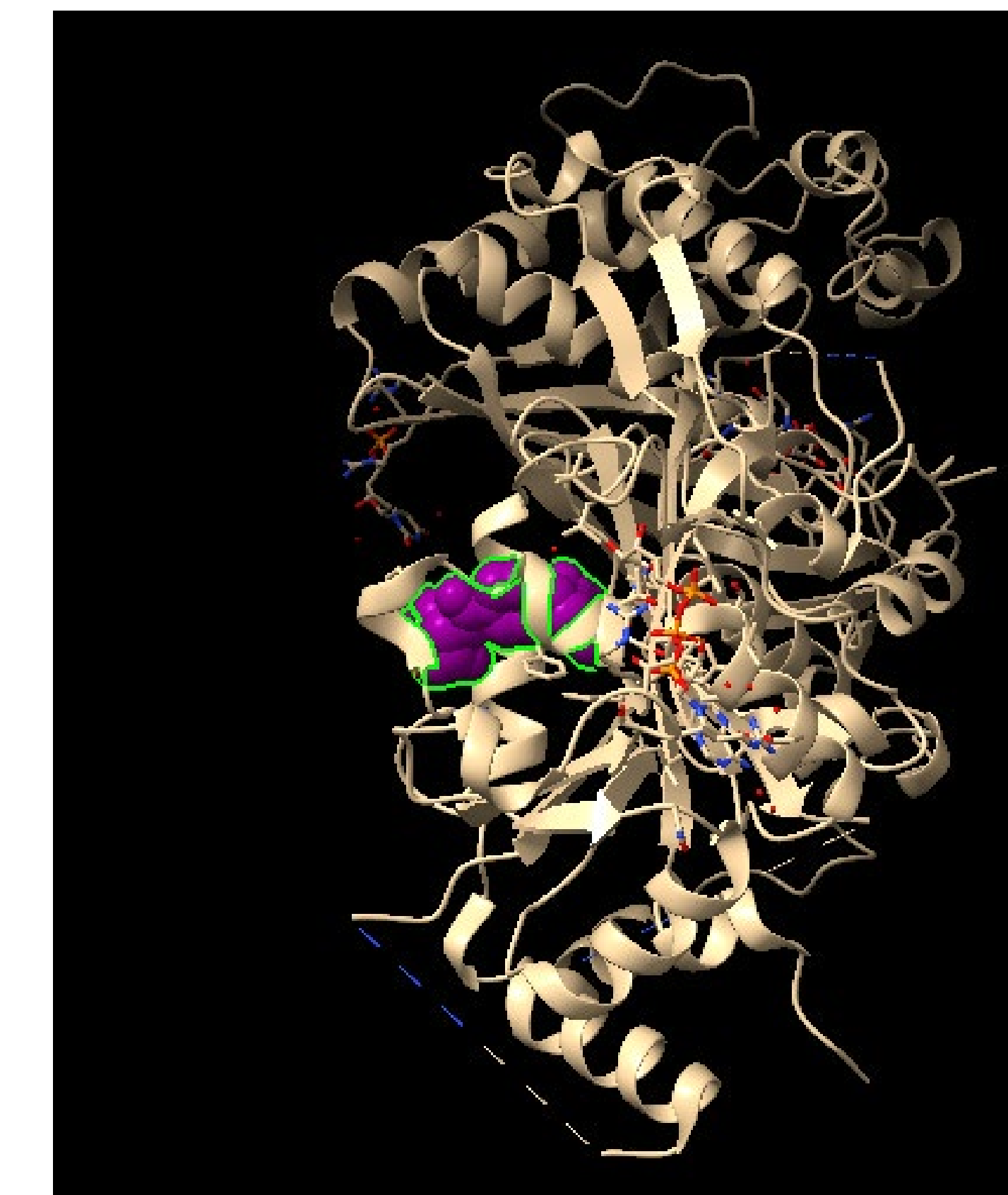
2. Actions

Actions>>Atoms/Bonds>>Delete



Highlight the Dihydrofolic Acid Ligand

1. Select>>Residues>>DHF
2. Actions>>Atoms/Bonds>>Atom Style>>Sphere
3. Actions>>Color>>Purple
4. Clear the selection (Control-Click in black background)

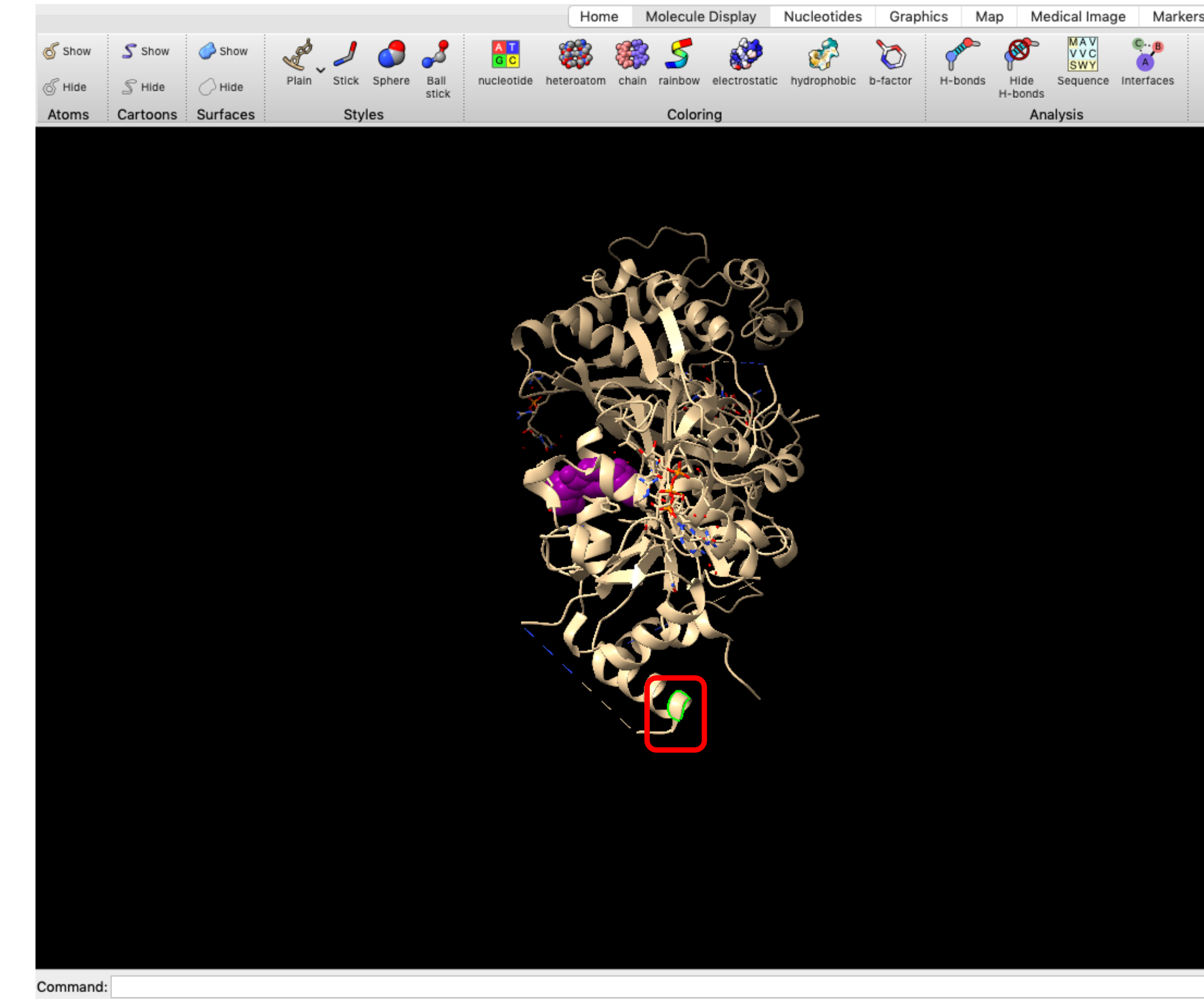


Selecting with mouse

Control-click at a point in the ribbon.
The selection is highlighted in green.

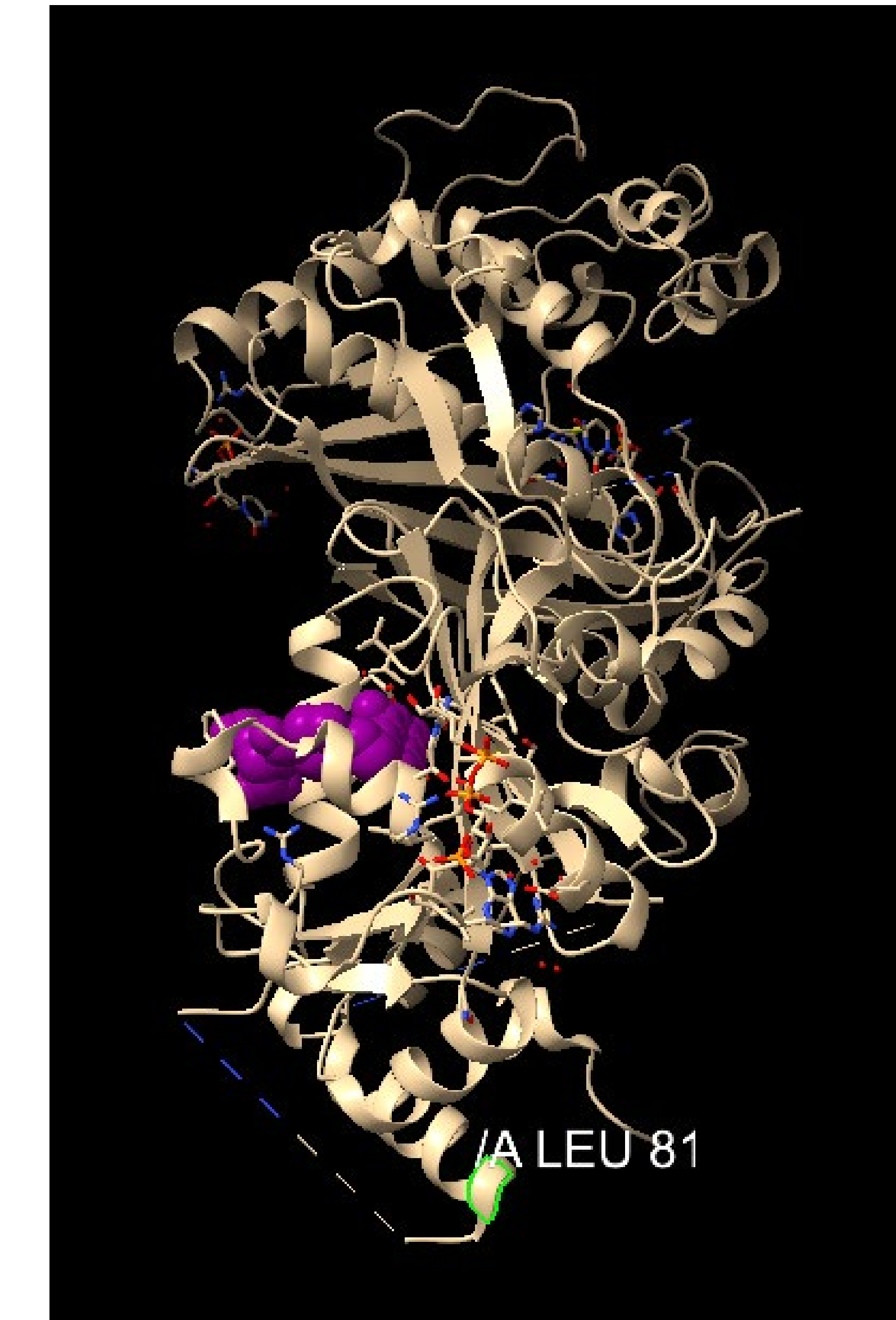
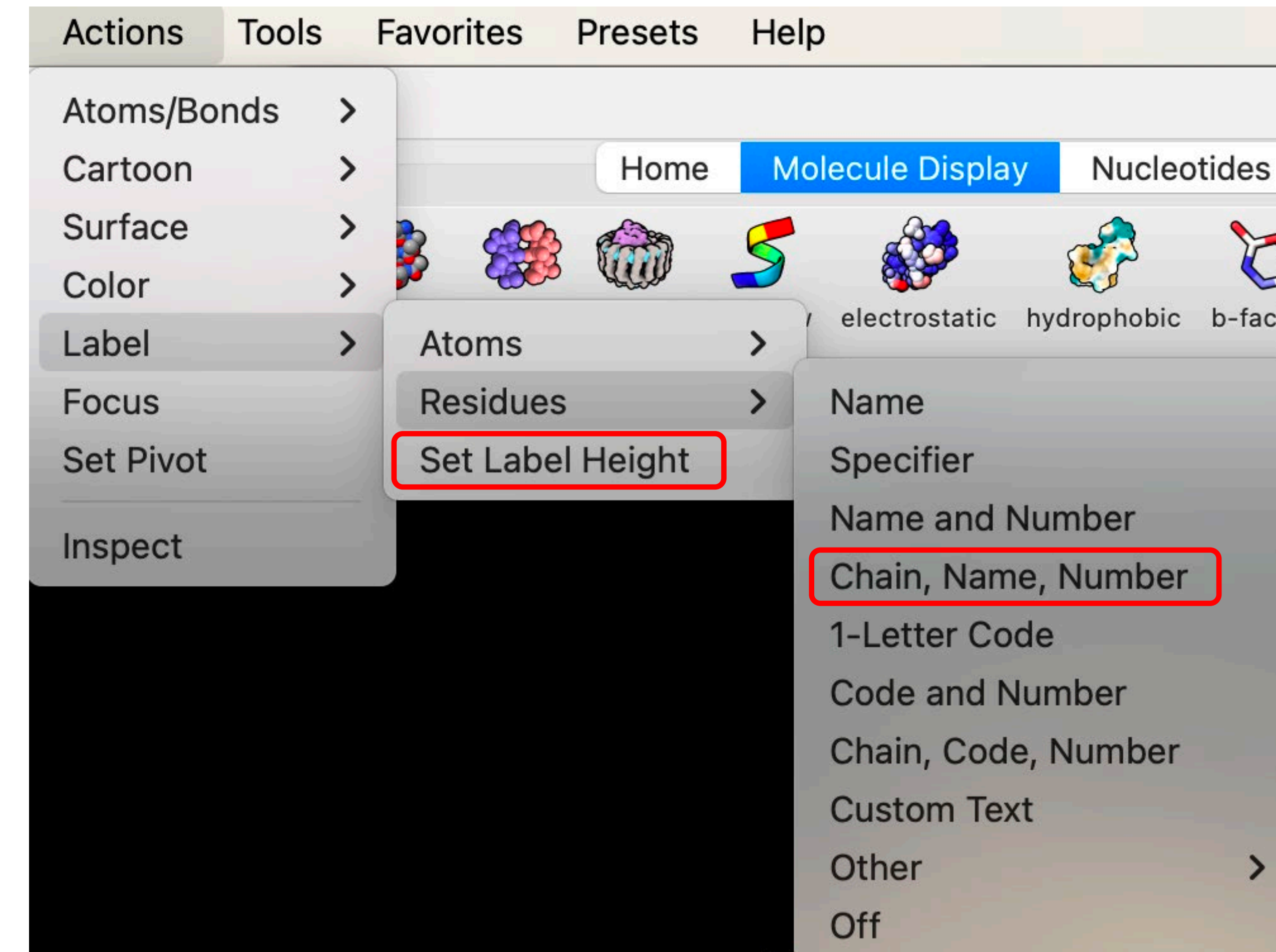
Additional selection operations:

- Control-shift-click adds to current selection
- **Typing up arrow in graphics window extends selection to domains in structure**



Add a label to the selection

1. Actions>>Label>>Residues
2. Select “Chain, Name, Number”
3. Actions>>Label>>Set Label Height
4. Set all label heights to 2.0 Å
5. Click “OK”

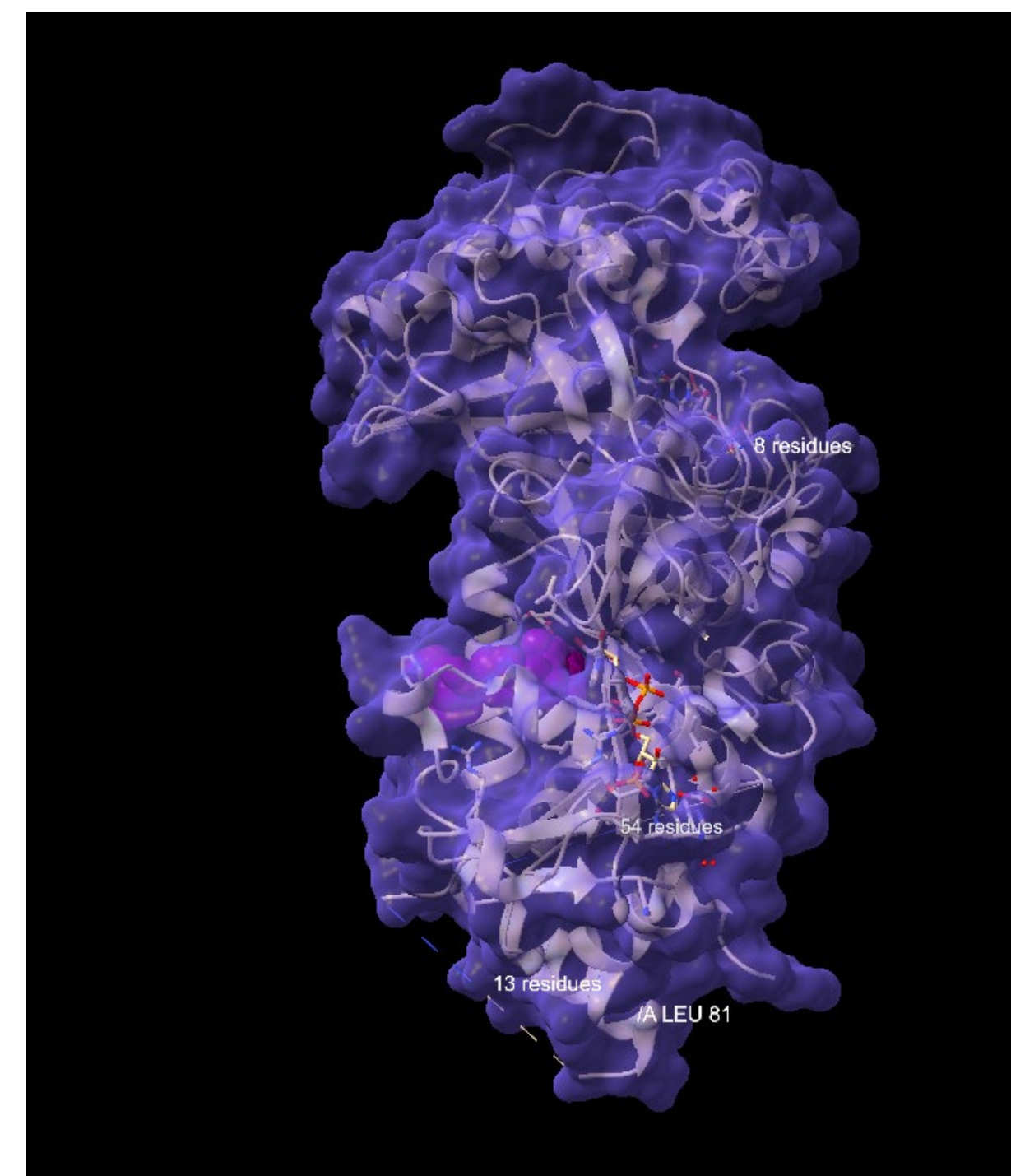
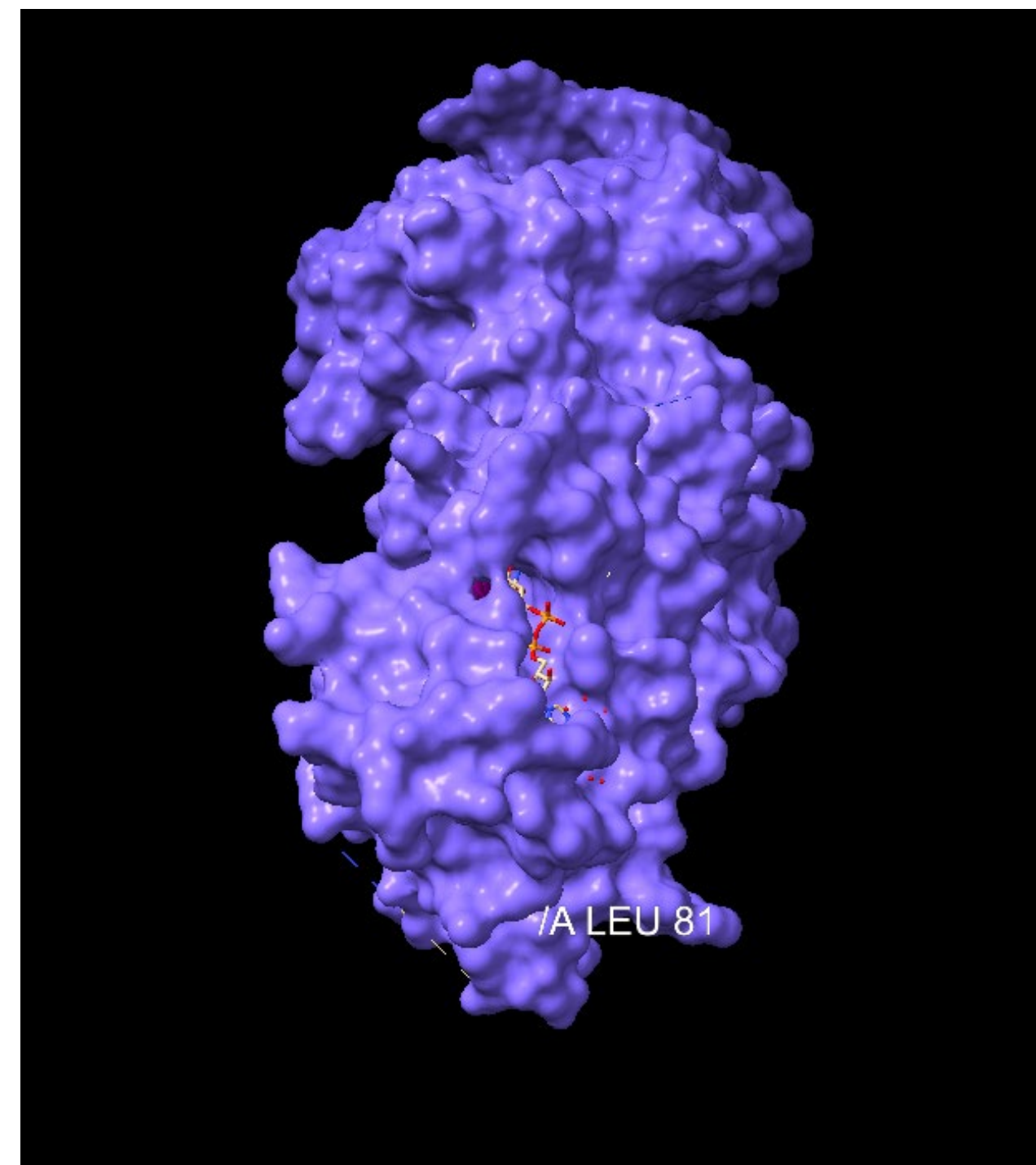
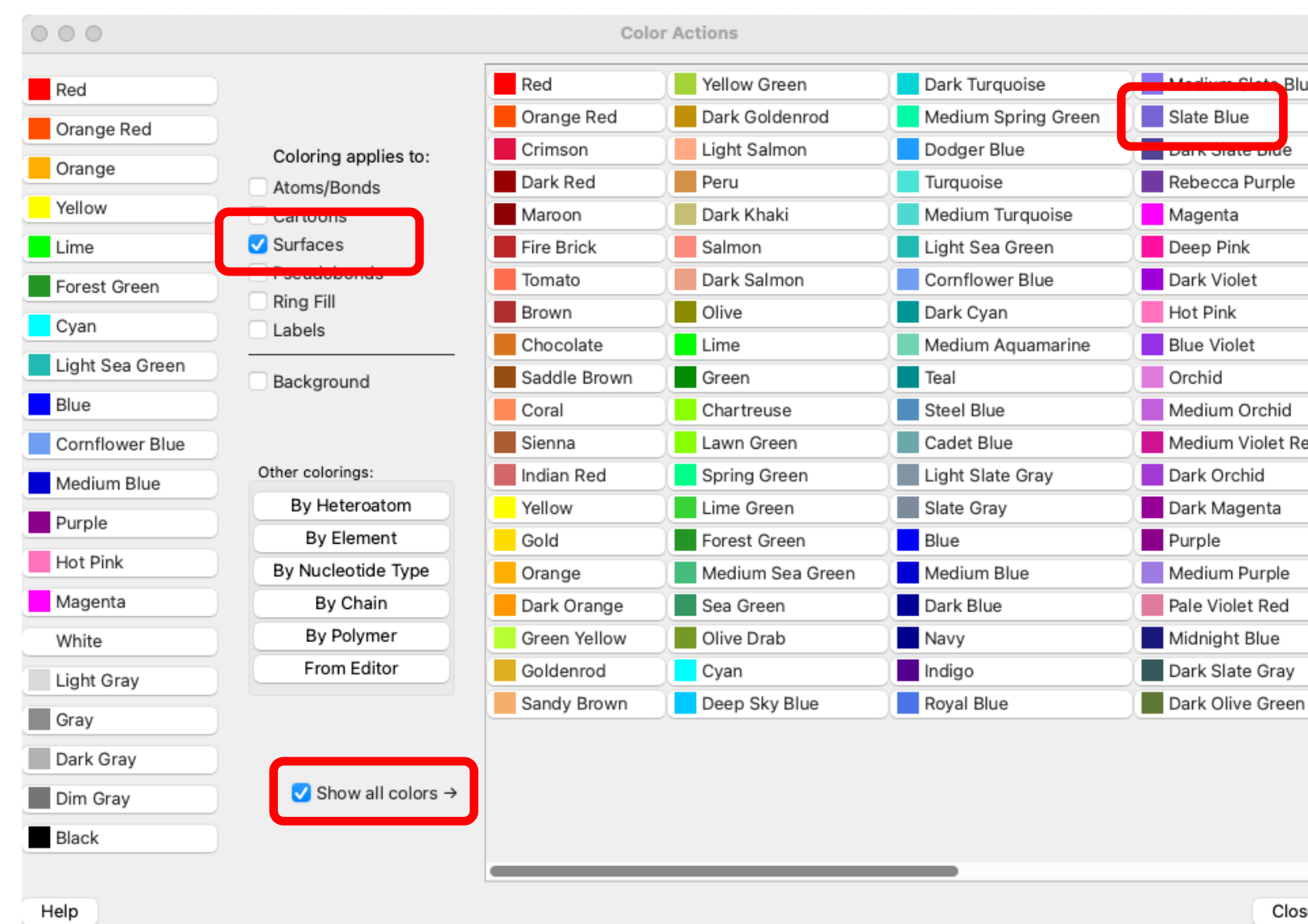


Add Surfaces

1. Control-click in background to clear selection.
2. Create a surface with:
Actions>>Surface>>Show

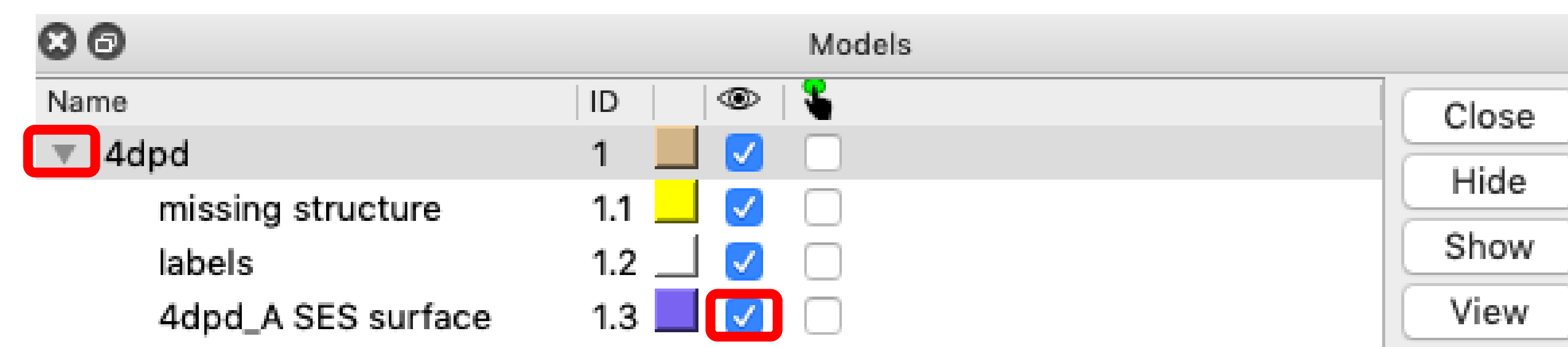
You will see a surface representation with bound ligands.

3. Actions>>Color>>All Options...
Color Applies to: (Select only Surfaces)
Check “Show all colors ->”
Click “Slate Blue”



1. In the Model Panel, click the little triangle next to “4dpd”.
You can turn on and off the various components of the scene with the check boxes under the eye icon.

2. Click the checkbox next to 4dpd_A SES surface to hide it.



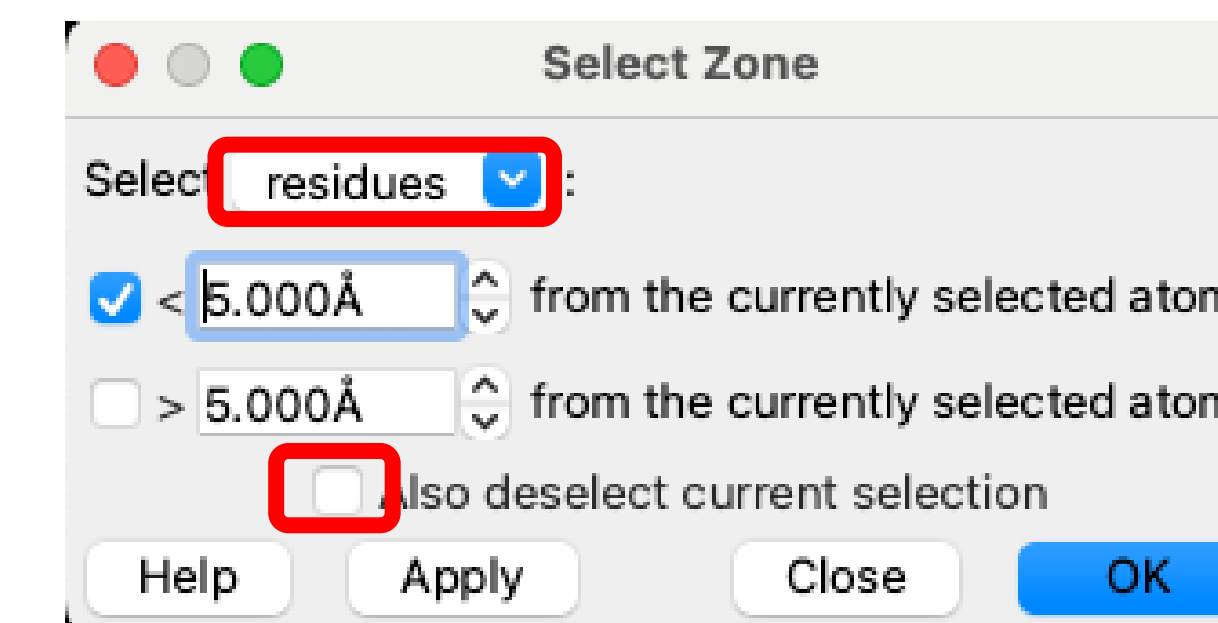
4. Actions>>Surface>>Transparency 50%

Find amino acids that interact with the DHF ligand

1. If showing, hide the surface: Actions>>Surface >>Hide

2. Select>>Residues>>DHF

3. Select>>Zone...



4. Change “Select” to “residues”

5. Click “Also deselect the current selection”

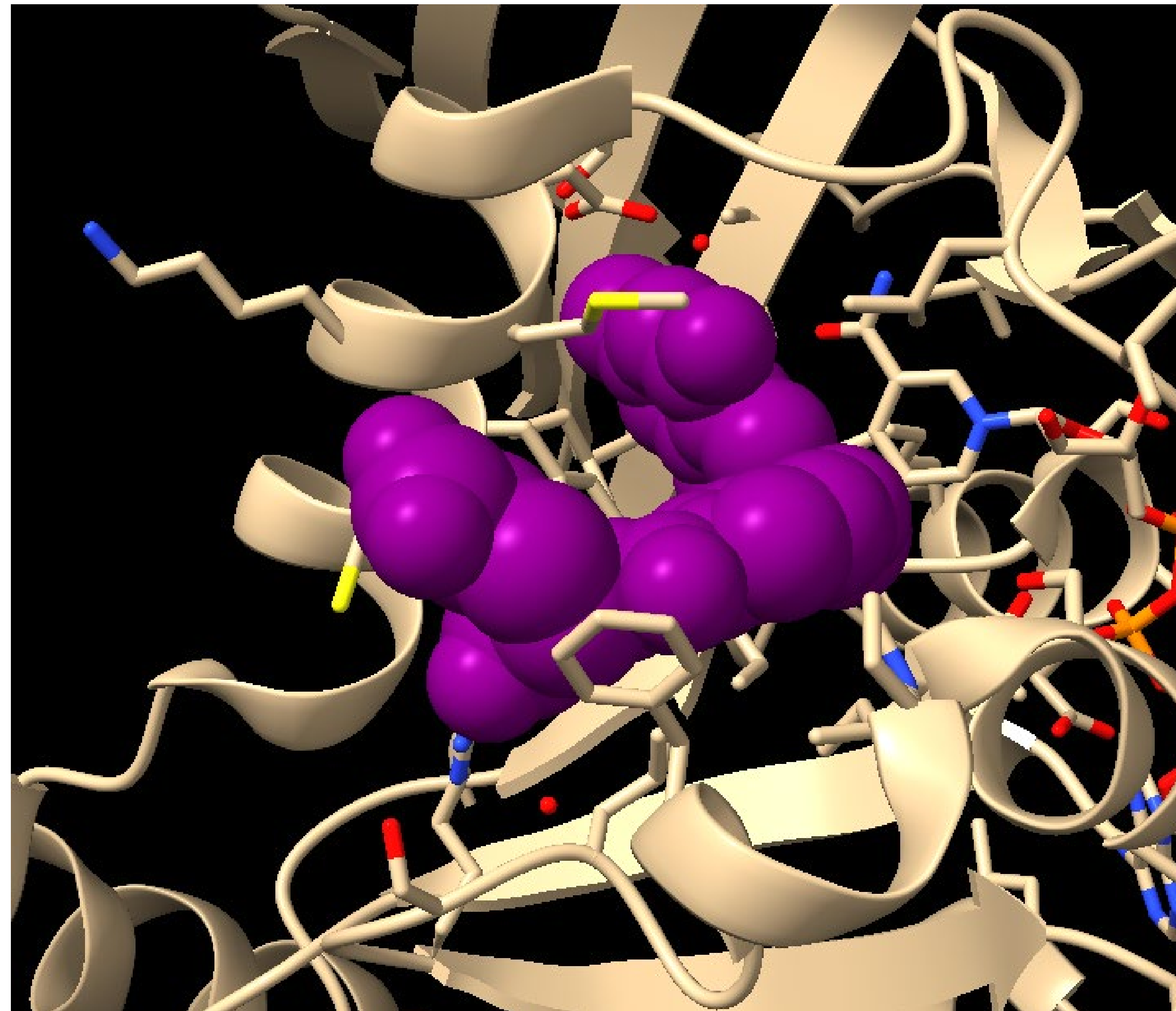
6. Click OK

Note that the residues less than 5 Å from DHF are now selected. Show their sidechains:

7. Actions>>Atoms/Bonds>>Show

8. Actions>>Color>>Cyan

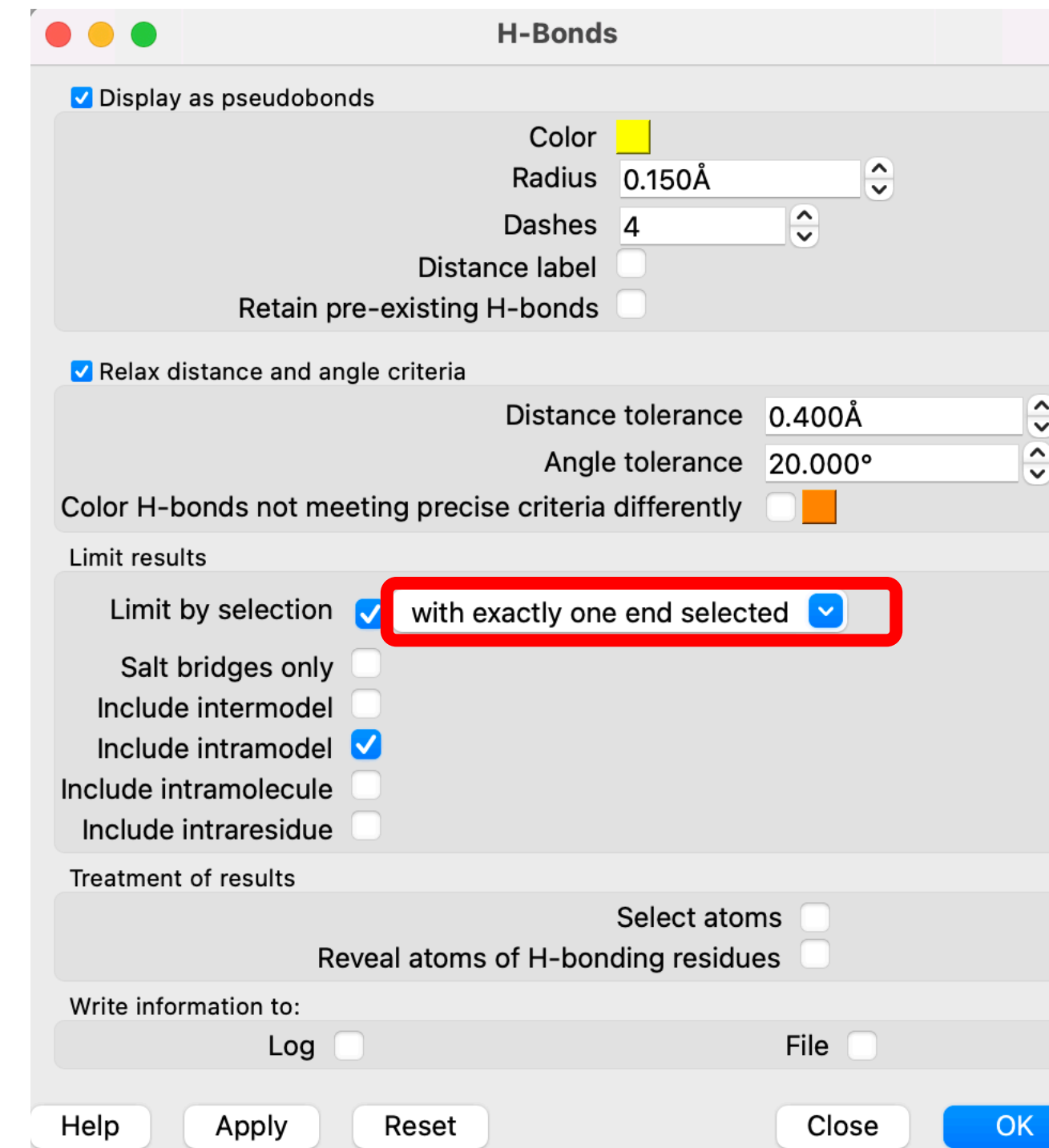
9. Clear the selection.



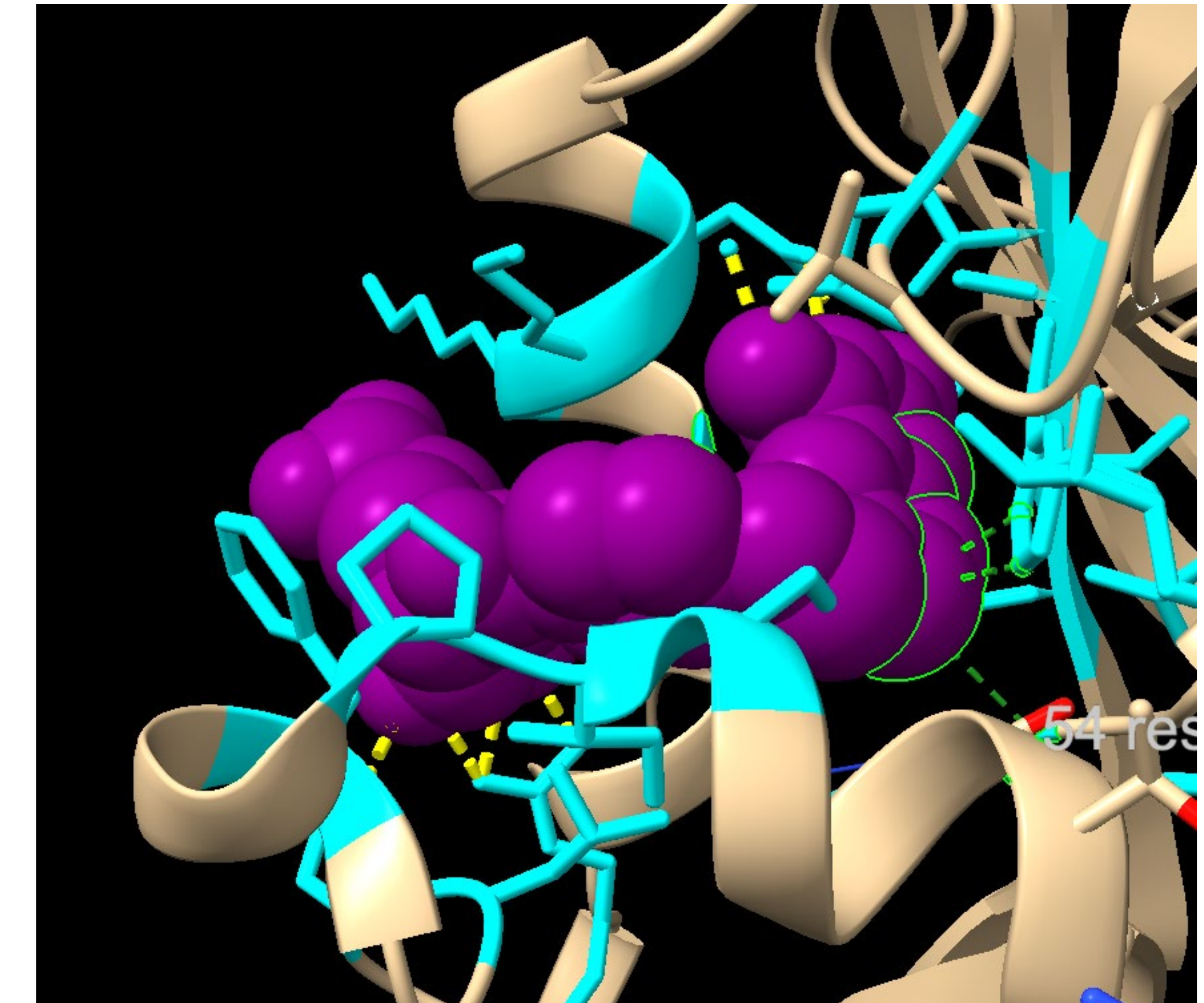
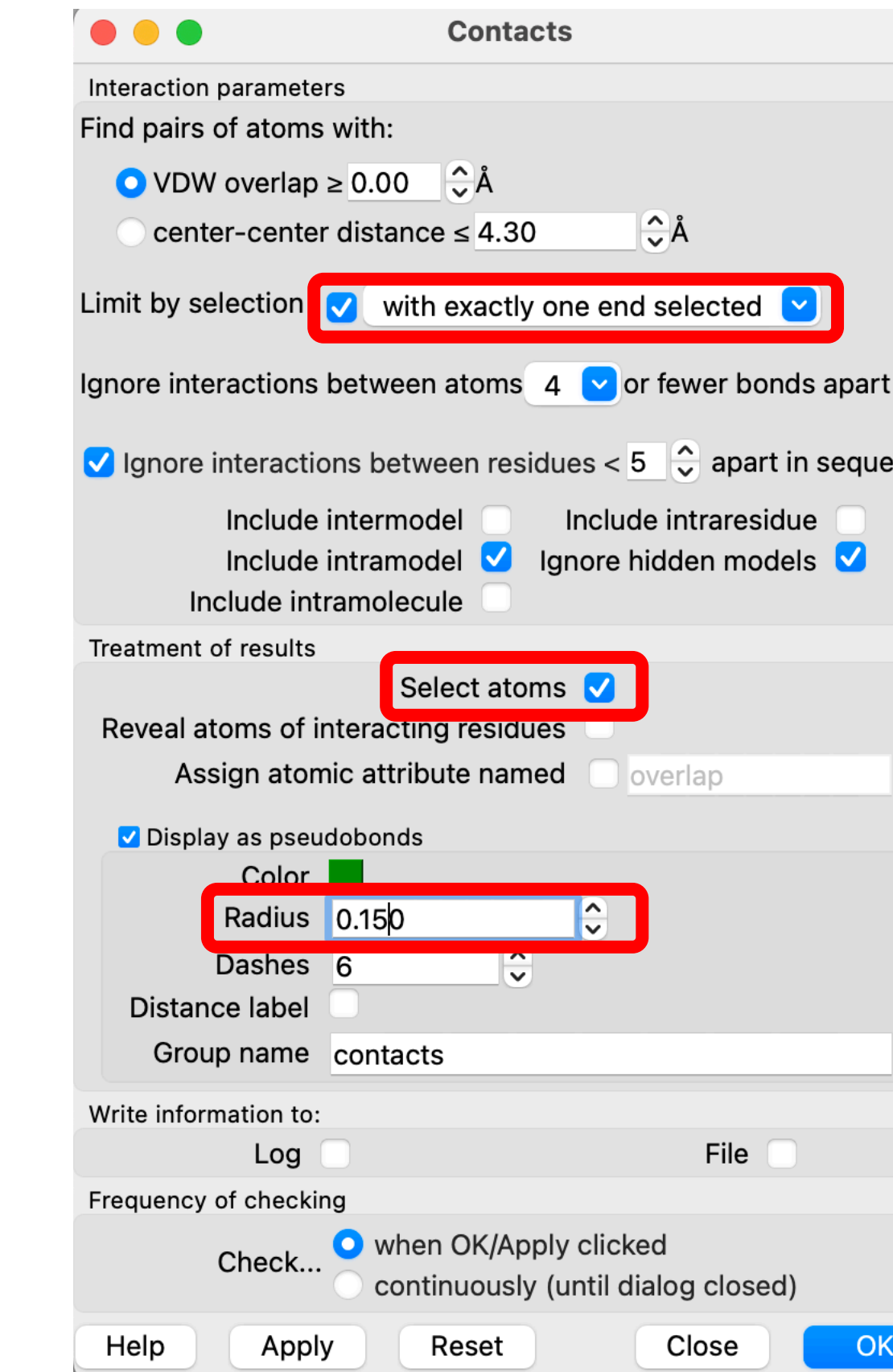
Find Hydrogen Bonds and non-Polar contacts near DHF

1. Select>>Residues>>DHF
2. Tools>>Structure Analysis>>H-bonds
3. Check on “Limit by selection” and set to “with exactly one end selected”
4. Click “OK”.

Note the H-bonds are shown with yellow dashed lines.



1. Tools>>Structure Analysis>>Contacts
 2. Check on “Limit by selection” and set to “with exactly one end selected”
 3. In the “Treatment of Results” section click “Select atoms”
 4. Set “Radius” to 0.150
 5. Click “OK”.
- Note the contacts are shown with green dashed lines.



Use the Sequence Viewer

1. Tools>>Sequence>>Show Sequence Viewer

2. In the “Show Chain Sequence” Dialog Box that appears you will see just one chain showing (/A: Bifunctional dihydrofolate ...)

3. Click “Show”.

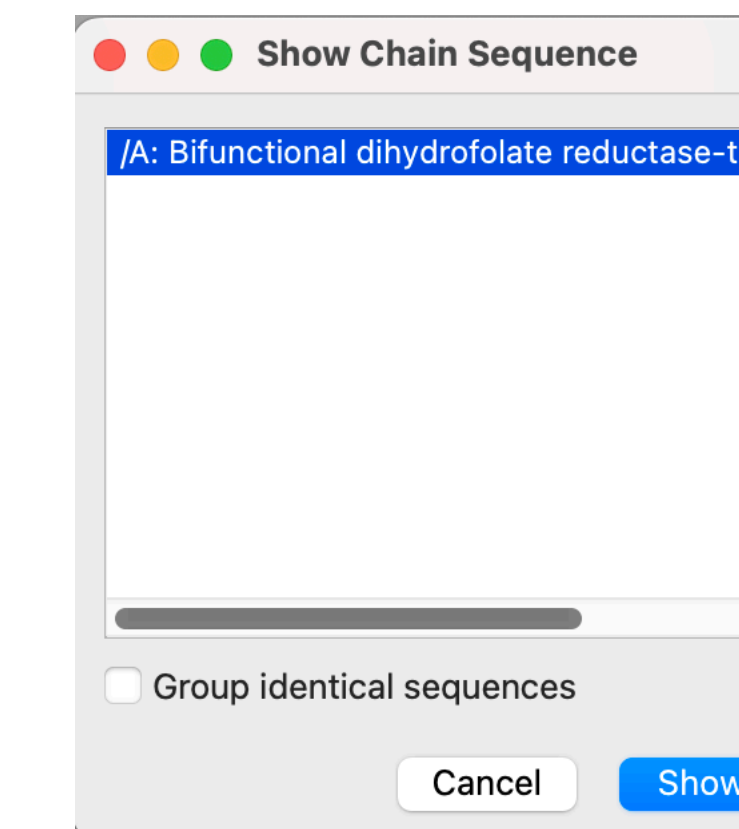
This brings up a new Sequence Viewer box showing the sequence corresponding to the selected chain.

This view of the sequence is live, i.e., linked dynamically to the structure in the 3D window. Note that two residues are highlighted in green. These show the current selection.

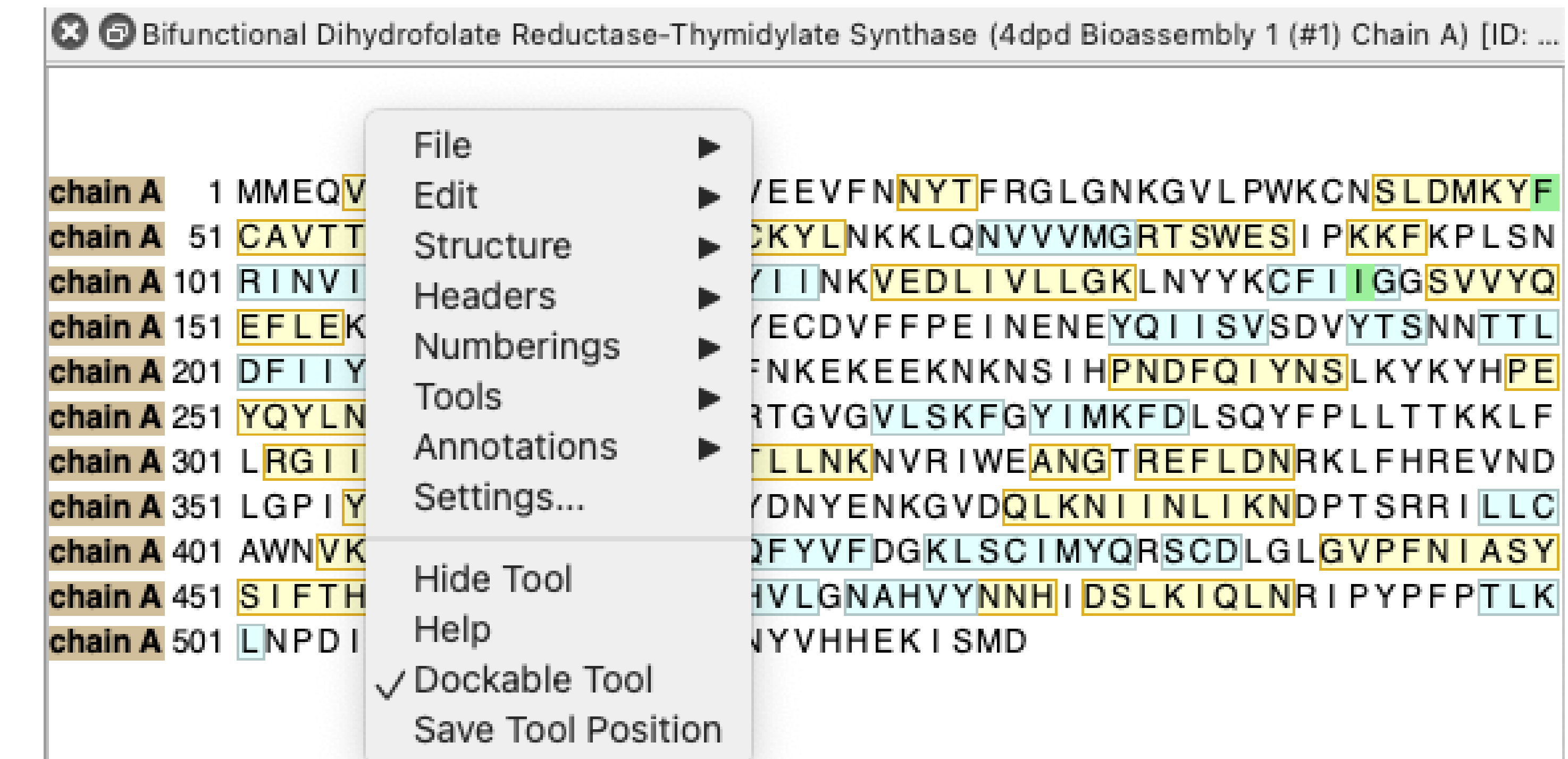
4. Place the cursor over one of these residues in the sequence viewer; a tool-tip will appear identifying it, e.g., /A PHE 58.

5. Click and drag within the sequence; the corresponding residues in the structure will be selected.

6. Select in the structure, e.g., with Ctrl-click, and the corresponding residues will be highlighted in the viewer.



Right-click in the sequence viewer to bring up a menu of additional options.



Align the structure to a human DHFR using Matchmaker

1. Fetch the PDB entry 1DHF

2. Delete Chain B by clicking “B” in the log to select it, then

Actions>>Atoms/Bonds Delete

Chain information for 1dhf bioassembly 1 #2	
Chain	Description
A B	DIHYDROFOLATE REDUCTASE

Delete the B-chain Folic Acid ligand and surrounding waters:

3. Put the cursor near the isolated ligand, then Ctrl-click and

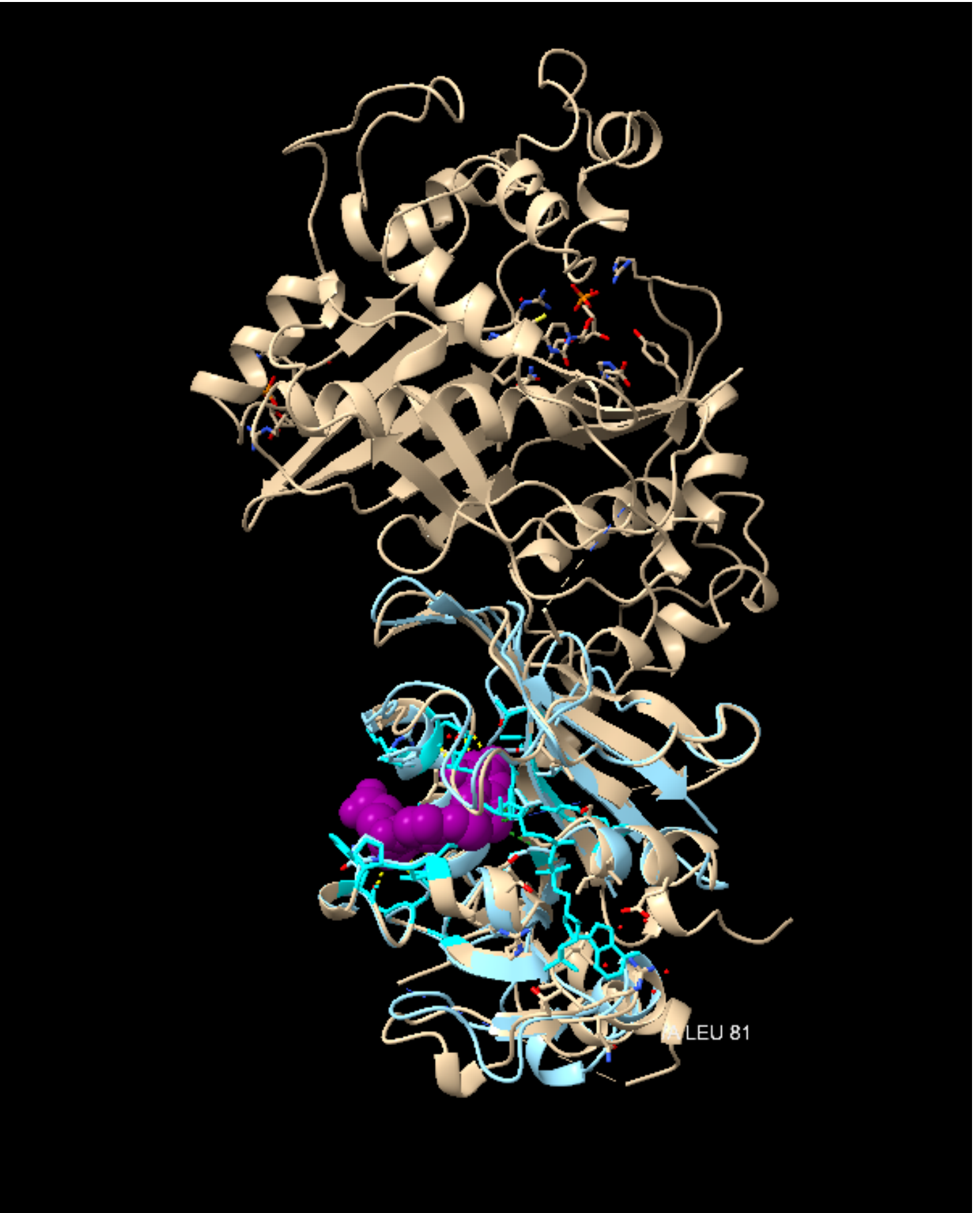
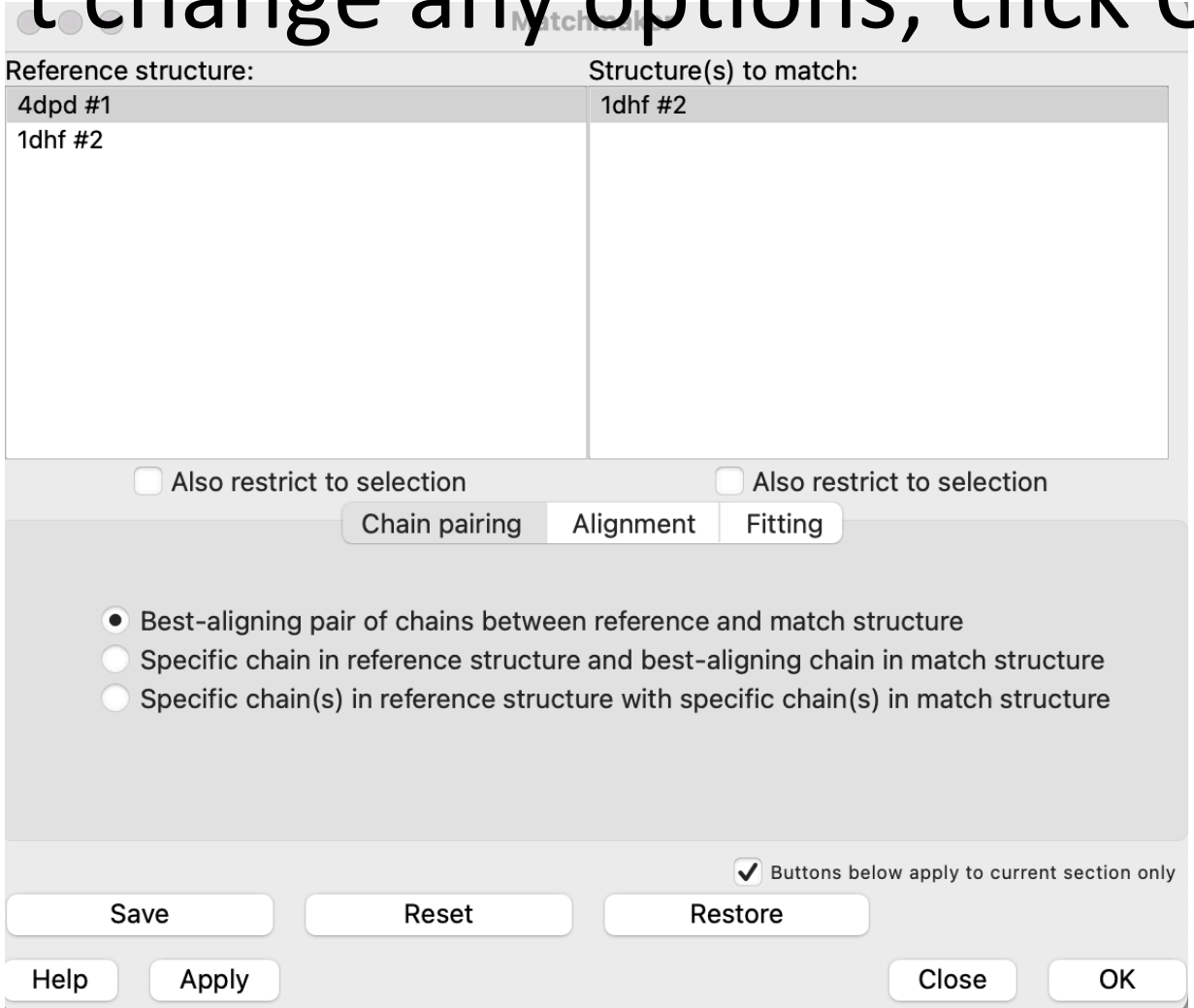
drag a square selection. Actions>>Atoms/Bonds Delete

Use the “Matchmaker” utility to align 1DHF with 4DPD:

1. Tools>>Structure

Analysis>>Matchmaker

2. Don’t change any options; click OK.



Note that 4DPD has a domain not present in 1DHF, and additional loops and helices. However, the structural homology is high near the DHF ligand.

Save the current session for later use

File>>Save...

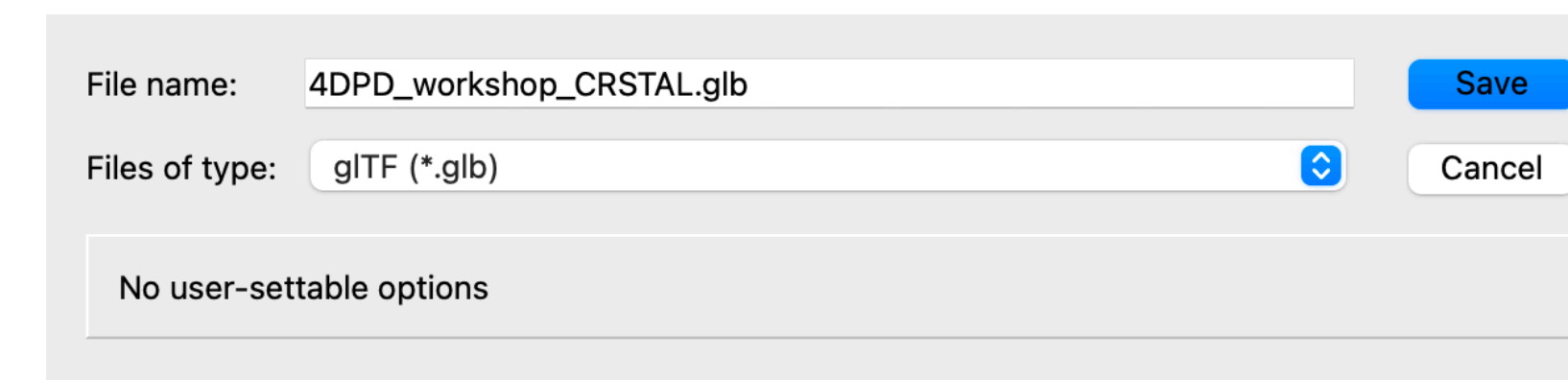
“Files of type:” choose “ChimeraX session (*.cxs)”

Enter a filename and click “Save”.

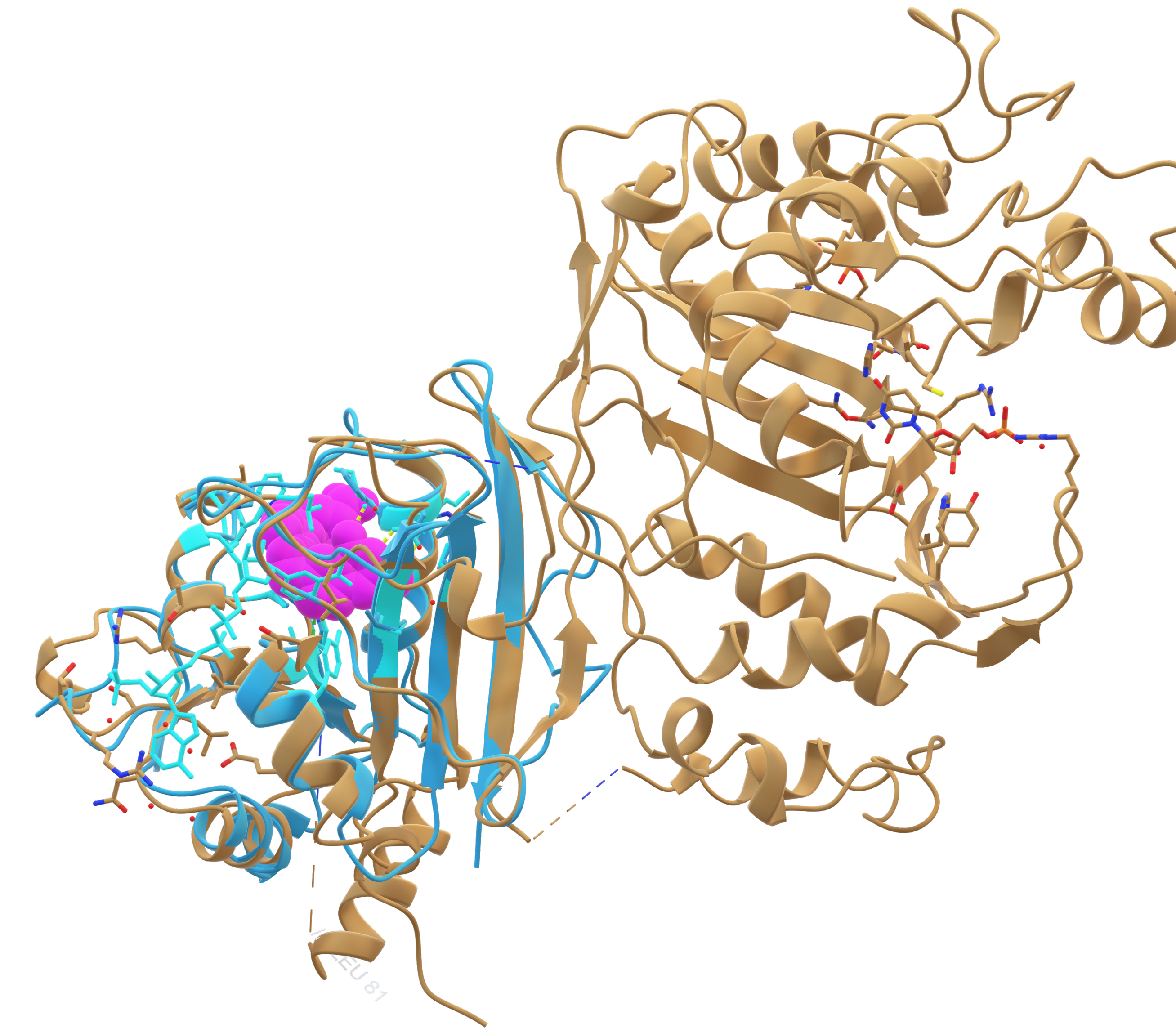
The .cxs file name extension is added for you.

Adding a live view into your presentations

- ChimeraX can save 3D image files in the .glb format. These can be inserted into PowerPoint presentations and Word documents. Note: this only works with the Desktop versions of PowerPoint and Word.



- Type in the command line: `color modify #* lightness 40`
- File>>Save...
- Make sure “Files of Type:” is “glTF (*.glb)”
- Give it a name including your initials, for example:
 - 4DPD_workshp_vr_PC.glb
- Click Save



Back to VR!

View DHFR binding site
and docked ligands in VR



Bonus exercise 1: LookSee application for Meta Quest Headsets

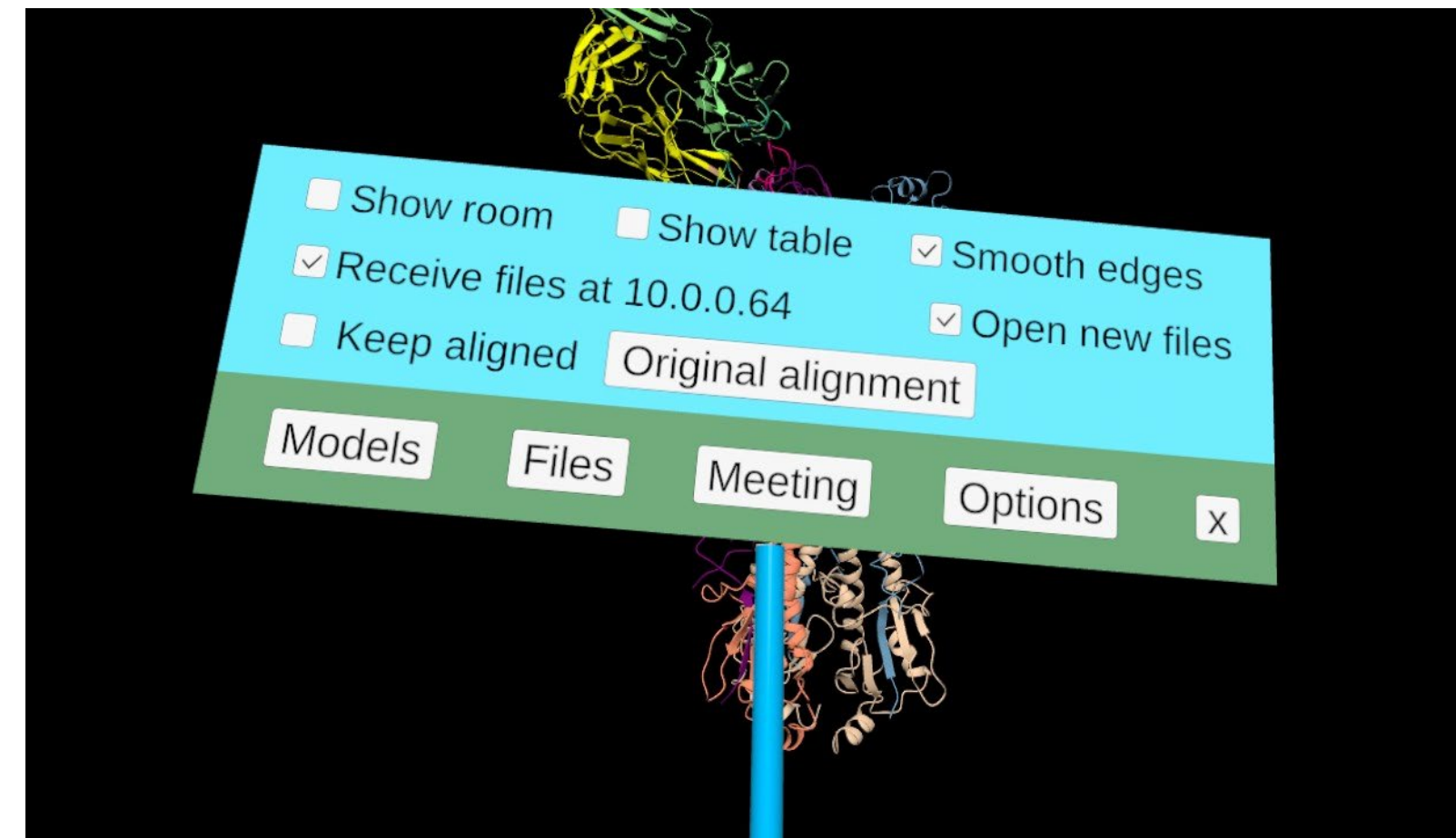
- ChimeraX can send a **graphics-only version** of the scene directly to a headset for viewing in the LookSee app. No Windows computer is required for this mode of viewing in VR.

- The ChimeraX computer and headset must be on the same network.

- In the headset, start the LookSee application

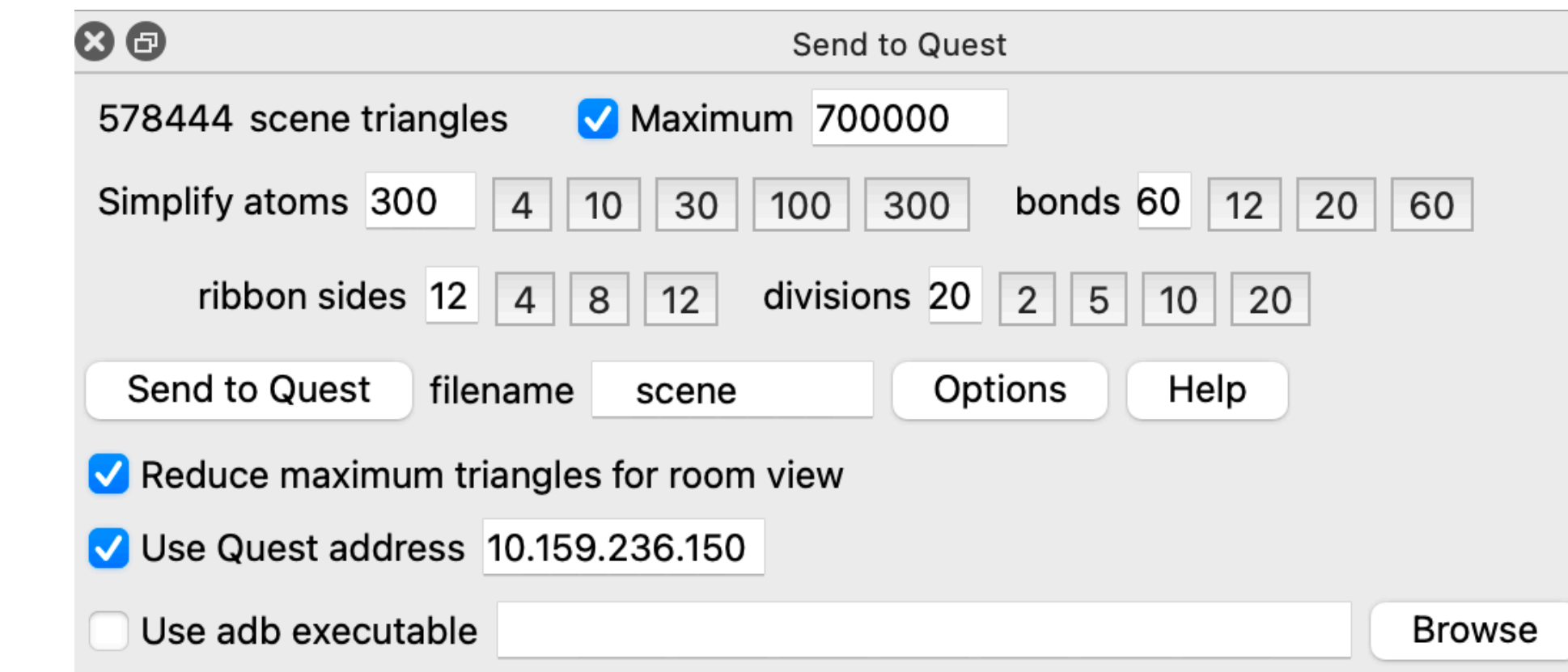
- Click to go into the Options pane.

- Click the checkbox "Receive at ..." and note the IP address.



Note: You can send to LookSee from any computer running ChimeraX.
The computer doesn't need to be VR capable. Works with Macs.

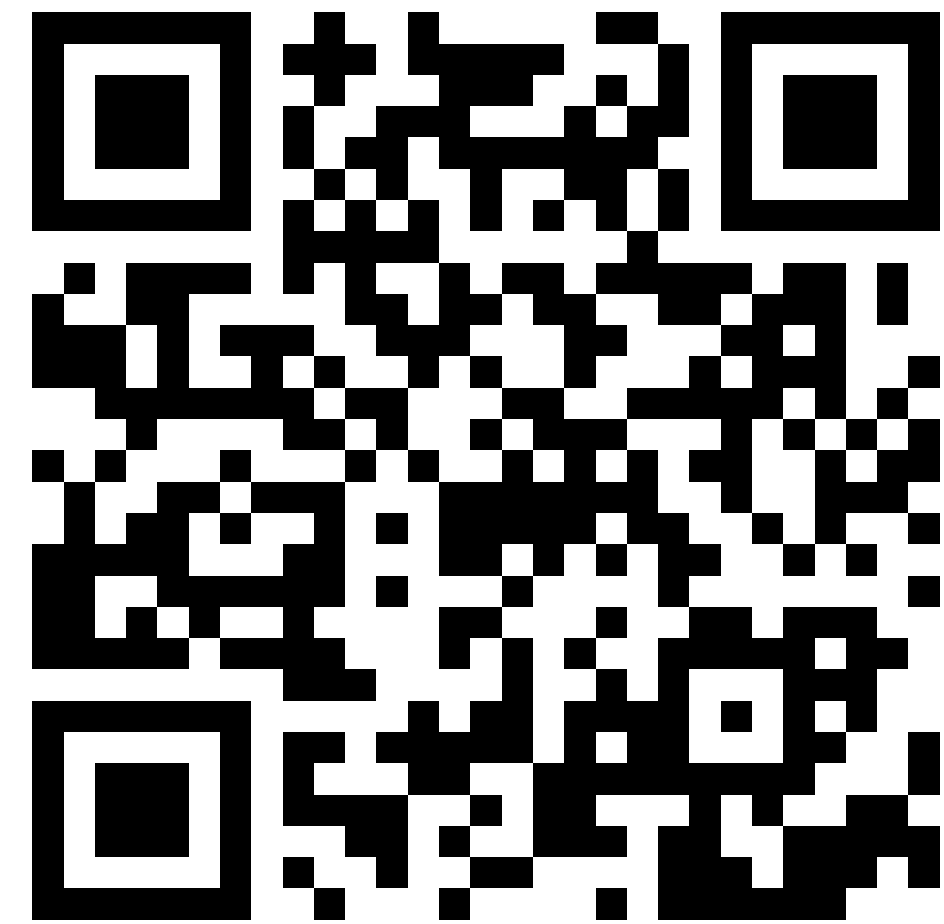
- On the computer, in the ChimeraX menu: Tools>>General>>Send to Quest



- Use this dialog box to simplify the number of scene triangles
- Connect to the headset
 - Click Options
 - Click "Use Quest address" and enter IP address noted in LookSee
 - Click "Send to Quest"
 - The scene will now be in the headset

Bonus exercise 2: Pathogen AR

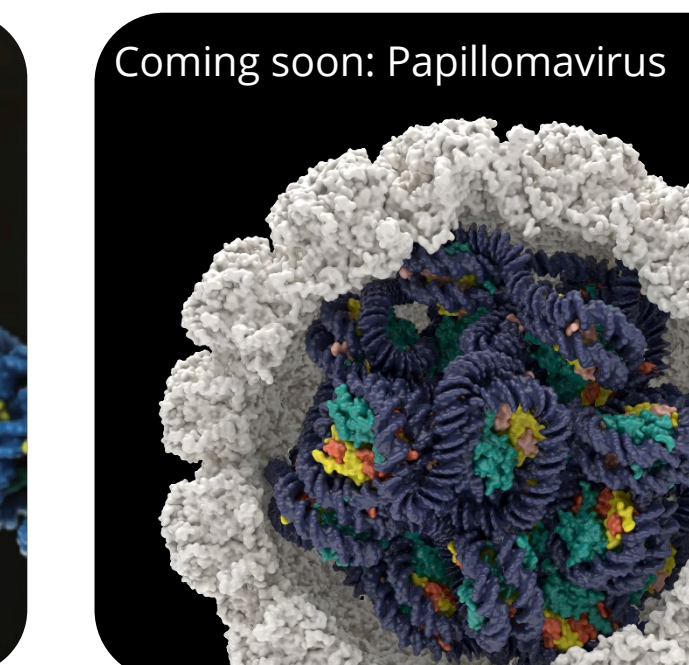
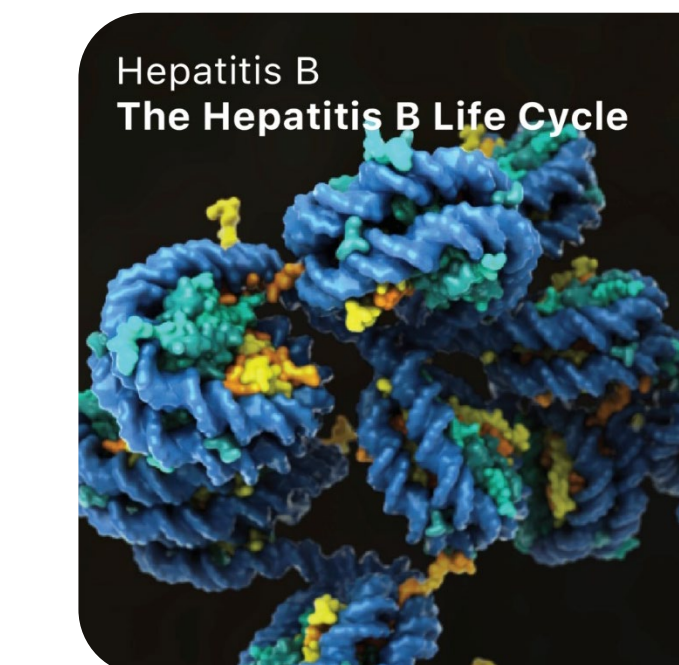
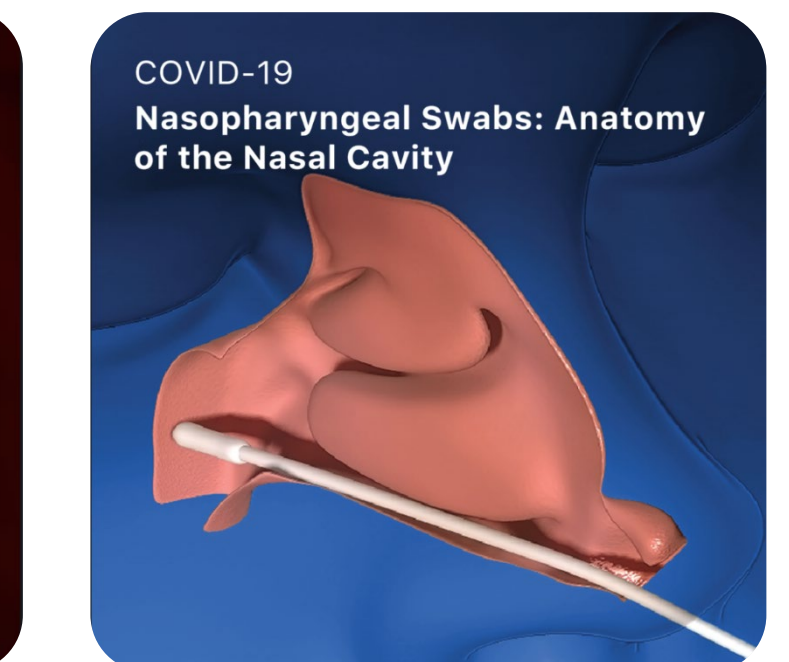
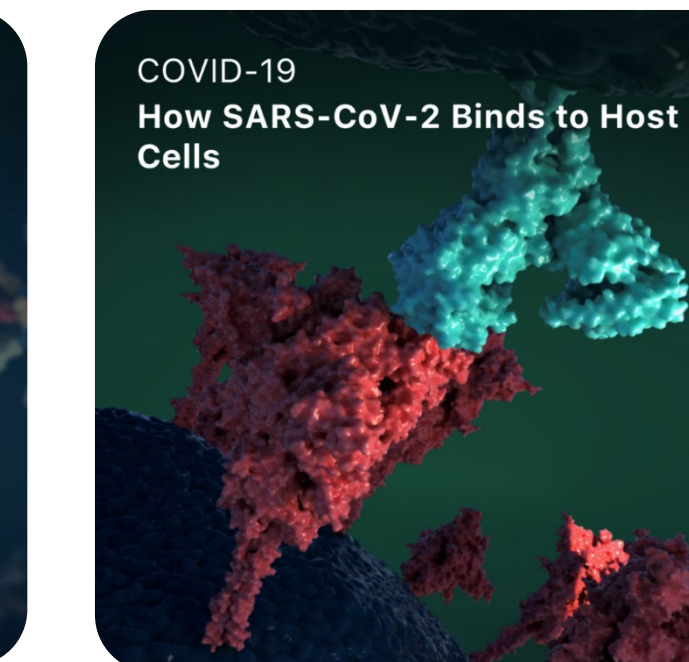
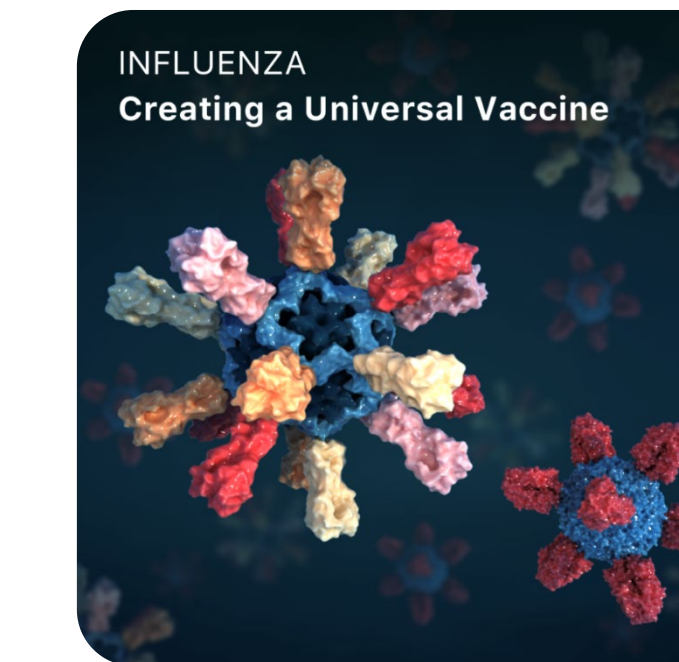
Download from Apple App store



Scan the QR code to
download the app



An augmented reality smartphone and tablet app with interactive stories about pathogens and pathogenic disease using touch gestures or a Merge Cube Device.



<http://onelink.to/k6sbpv>



Bonus exercise #3: NIH 3D WebXR

- Open the browser app in the Meta Quest headset
- Navigate to 3d.nih.gov (try using voice commands!)
- Find any model page
- Select the “WebXR Beta” button to open the XR view

NIH National Institute of Allergy and Infectious Diseases

NIH 3D

Models Search by title, ID, keyword...

Discover Submit Collections FAQs BioArt

Discover / 3DPX-023329

306C7B3 Antibody

Generated by NIH 3D workflows using data provided by [Devarsh Aswin](#)

Created: 2/21/26 Submitted: 2/2

3D View WebXR Beta



fold_2026_01_29_21_17_306c7b3_trial_1_model_0-ribbon-secondary-vis_NIH3D

Ribbon representation colored by secondary structure (a-helix: blue, B-sheet: red, coil: yellow). Not intended for 3D Printing

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[How to cite this NIH 3D entry](#)

35 5 Version History

Category: Biomacromolecules

Description