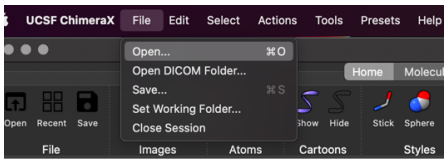
Chimera X

Open the file with the structure

open PDB ID ***open 5O1Z*** (Nrd1, RNA)

open Desktop/Name.pdb(mrc,cxs,etc.)

File -> Open

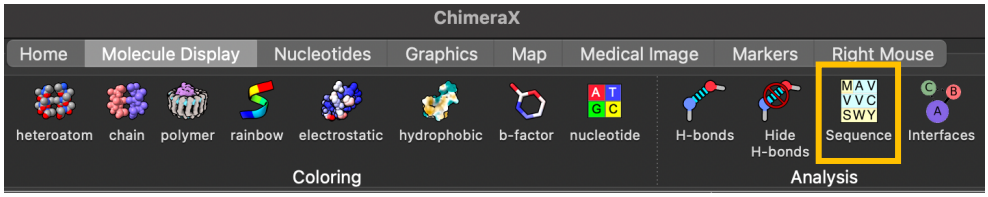


Movements (using mouse)

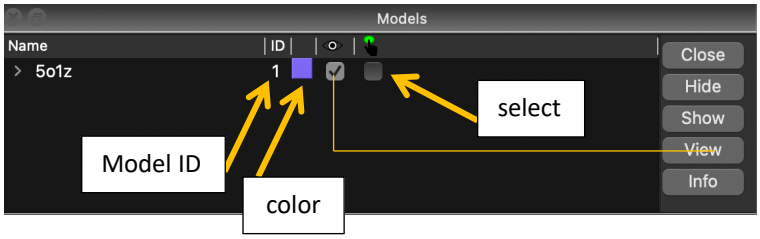
Left-click-holding - rotate the structure about the vertical and horizontal axis
Right-click-hold - move the centre of the protein about the screen

Sequence viewer

- **Tools** -> **Sequence** -> **Show sequence viewer**
- **Log window** -> Click on the link in the Chain information table
- **Molecule Display (Analysis section)** -> **Sequence**

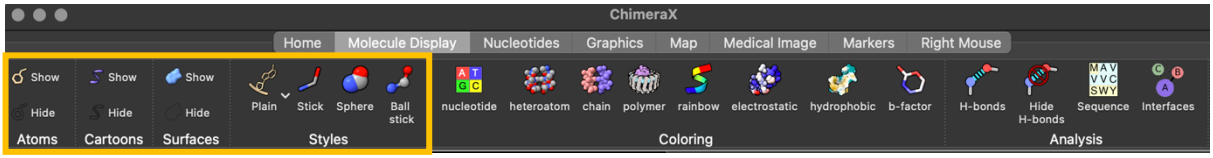


Model panel



Structure depiction

- Actions - > Atoms/Cartoon/Surface…hide/show
- **show** atoms/cartoon/surface
  hide atoms/cartoon/surface



Select

- Ctrl/(Ctrl+Shift) + LeftMouse
- Select -> Chains, Chemistry,…
- Sequence viewer
- ***sel***

Nomenclature

#1 => model ID ***sel #1*** (model/structure 1)

/A => chain ***sel #1/A*** (model/structure 1, chain A)

:400 => residue number

sel #1/A:464 (one residue nr. 464) **- show atoms**

sel #1/A:373-414 (residues from 373 to 414)

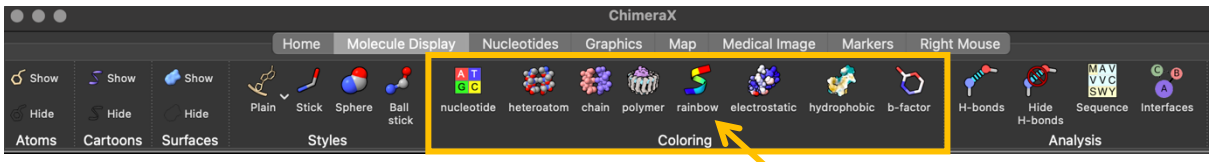
sel #1/A: 373-414 &:arg (residues from 373 to 414 that are arginines) **- show atoms**

sel #1/A:378, sel #1/A:342, sel #1/A:376 (residue 378, 342, 376) **- show atoms**

:arg => all arginines in the selection

@ => atom specifier (e.g. @ca). ***sel #1/A@ca*** or ***sel #1/A:400-450@ca***

Color



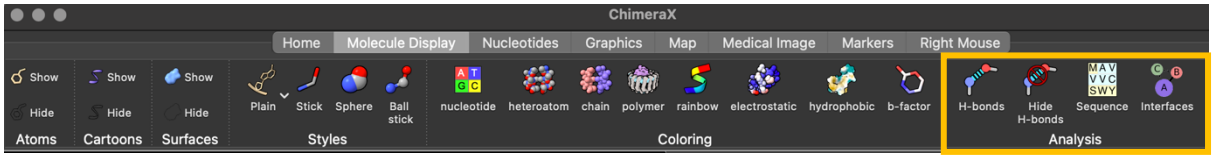
- Actions -> Color
- ***color*** [what] [color] ***color #1/A red***

from N-term to C-term

Zoom

- ***zoom*** **1.5**
- mouse -> spinning the middle wheel

Hbond



- Tools -> Structure analysis-> H-Bonds
- ***hbonds*** ***hbonds*** or ***hbond #1/B*** *or* ***hbond ligand***
- ***hide*** hbonds

Contacts

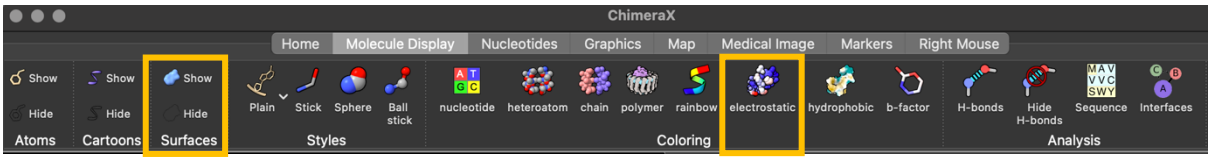
- Tools -> Structure analysis-> Contacts
- ***contacts***

contacts #1/A@C* restrict #1/B@C* distance 3.8 reveal true name vdW

Distance/angles

- Tools -> Structure analysis-> Distance
  ctrl+shift and pick the two/three atoms of interest
  (Model panel -> distances + distances labels – editing)

Surface



- Actions -> Surfaces-> hide/show
- Tools -> Depiction -> Surface Color ….by electrostatics -> Key. (remove from model panel)

NMR vs Crystallography

NMR -> bundle of structures (***open 2li8***)

Tools -> Structure analysis -> Matchmaker

Crystalography -> ***delete*** solvent

Hide/delete

- Actions -> Atoms/Bonds -> Delete
- ***del*** ***del #1/A:400-450***
- Actions -> Atoms/Bonds, Surface,… ->Show/Hide
- ***hide*** [what]

Save

File -> Save (cxs, pdb,…)

Tutorials

https://www.cgl.ucsf.edu/chimera/tutorials.html

https://www.cgl.ucsf.edu/Outreach/Tutorials/GettingStarted.html