1. **What is in the PDB file that I am looking at**?
* Upload/fetch file >> Presets >> Interactive 1 >> (each polymer chain is colored in a different color)
* Figure out what each chain represents >>
	+ Type PDB ID in top search box ([www.rcsb.org](http://www.rcsb.org)) >> Open structure summary page >> Read about contents by chain ID Go to Chimera graphical display >> mouse over chains and match chain ID with that on structure summary page
1. **To Select**: See selection (the selected atom, residue, chain etc.) highlighted with a green halo
	1. ***An atom(\*)***
* Left click on atom in graphics display with Control button pressed
	1. ***A specific residue***
* Left click on any atom of residue (see above\*) >> press up arrow OR
* Select residue from sequence based on chain ID and residue number
	+ Favorites >> Sequence >> *See new window with sequence* >>
	+ Mouse over amino acid sequence to see chain ID and residue number >> Click-drag on one or more specific amino acid residues in sequence window to select them
	1. ***All residues of a type(#)***
		+ Select >> Residue >> Standard (or Non-standard) >> select a specific one (or all) OR
		+ Select >> Residue >> Amino acid category
	2. ***A chain***
		+ Left click (with Control pressed) on any atom of residue (see above\*) >> press up arrow (pressing it once *selects residue*, twice *selects secondary structural element* and thrice *selects chain* etc.; clicking down arrow reverses these selections) OR
		+ Select >> Chain >> select Chain ID (A or B or C etc.)
	3. ***A specific type of residues within a or chain or a selected group of residues/chains($)***
* Select chain/group (see above) >>
* Select >> Selection Mode >> Intersect >> Select specific type of residue (see above #)
* Reset selection mode >> (Select >> Selection Mode >> Replace) for further selections
	1. ***A zone (%)***
* Select a residue or chain (as above) around which to explore >> Select >> Zone >>
* *New window opens* >> input the distance within which all residue should be selected >>
* Input/select options to select zone (atoms/residues within specified distance)
1. **To See or Hide**:
* Select residue(s)/chain(s) >> Actions >> Atoms/Bonds or Ribbons or Surface >> Show or Hide
1. **To explore interactions within or between polymer chains**:
2. ***Find H-bonds***
* To find all H-Bonds in structure: Tools >> Structure Analysis >> FindHBond >> OK
* To find ones in a selected set of residues: Tools >> Structure Analysis >> FindHbond >> Check on “Only find H-bonds” options (with at least one end or both ends selected) >> OK
1. ***Find hydrophobic interactions***
* Select >> Residue(s) (either in entire structure or within a selected set (see above $ or %)) >>
* Amino acid category >> hydrophobic >> Action >> Atoms/Bonds >> Show >>
* Examine residues >> Mouse over atoms or Left click on them to identify them
1. ***Find charge-based interactions***
* Select Amino Acid category# >> Negative >> Actions >> Atoms/Bonds >> Show >>Actions >> Color >> select color 1
* Select Amino Acid category# >> Positive >> Actions >> Atoms/Bonds >> Show >>Actions >> Color >> select color 2
* Visually locate pairs of color 1 and color 2 amino acid side chains within (~4-6 Å) of each other >> do closer analysis
1. ***Find pi-pi interactions***
* Select Amino Acid category# >> Aromatic >> Actions >> Atoms/Bonds >> Show >>
* Examine location and orientation of aromatic rings >> Identify sandwiched, edge-to-face, displaced interactions
1. **To compare structures**:
* Upload/Fetch PDB entry of interest >> Orient/understand all components (polymer chains, ligands) >>
* For complex structure, click on Presets >> Interactive 1 >> this colors the chains in the polymer >>
* Upload/Fetch one or more PDB entries to be compared >> Tools >> Structure comparison >>
* Matchmaker >> *New window opens* >> Click to select pairs of PDB IDs - Reference structure (in one column) and Structure(s) to match (in the other) >> OK >> Review the graphics window to see match
1. **To measure distances**:
* Select two atoms – press Shift + Control + Left click on the atoms in the graphics window >>
* Tools >> Structure Analysis >> Distances >> Create - Distance reported in graphics and new window
1. **To label structures**:
* Tools >> Utilities >> 2D Labels >> *New Window opens* >> Left click on desired label location >>

Write text (select font, color etc.)>> Show or hide label and move to suitable location OR

* Actions >> Label >> select general or Residue options >>

Edit label color options from Actions >> Color >> All Options >> select Label options in new window

For a quick overview of key functions of UCSF Chimera check out the following short videos:

* + - 1. Basics (<https://www.youtube.com/watch?v=hQxKYSUdiD8>)

- how to open a file from the PDB in the software, interact with it, save images and close the software.

* + - 1. Menus (<https://www.youtube.com/watch?v=ZICQW3LBdpw>)

- how to select, display, color and label specific residues and chains in different representations

* + - 1. Selections (<https://www.youtube.com/watch?v=HRPVmRD5e1U>)

- how to select specific residues from the graphics window or in a specific polymer chain to visualize and explore

* + - 1. Structure analysis (<https://www.youtube.com/watch?v=eLxhKc7Ljjk>)

- how to explore the interactions of a given residue or ligand with its neighboring atoms, measure distances, angles etc.

* + - 1. Structure comparisons (<https://www.youtube.com/watch?v=oThN3LG8LQU>)

– how to compare and visualize the structures of two related proteins/domains.