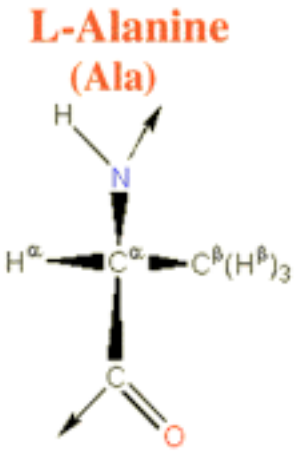
Exercise 21

This exercise will allow you to use Bio.PDB to analyze the 3rif.pdb file that you previously looked at in ChimeraX. Write code that can perform the following:

1. Print out the name of each chain in the structure along with the number of residues and atoms that belong to each chain.
2. Iterate through all of the residues in the structure and identify all of the unique residue names (and print them out). A set is a useful data structure for holding the unique residue names.
3. Iterate through all of the atoms in the structure and identify all of the unique elements and atom names (and print them out). What is the difference between element and atom name?
4. IVM is the residue name for ivermectin. Ivermectin is a ligand that binds the protein and not an actual protein residue. Determine what is unusual in the residue object for IVM that you can use to determine it isn't an amino acid. Use this info to find all the other residues that are also not part of the protein. What are their names?
5. Determine which chain each of the ivermectin residue belongs to. Which chain does not have a ivermectin residue? Which chain has multiple ivermectin residues? (There is nothing biologically significant about this)
6. The 20 amino acids have a very common backbone and thus naming system for some of the atoms that make it up. Check to see if all of the amino acids have an alpha Carbon and a beta Carbon. Hint: one of the 20 amino acids lacks one of these. How come?



7. Create a function that takes in two residues and returns the minimum distance two atoms are from each other within these two residues (i.e. one atom must be from the first residue and the second atom must be from the second residue)
8. Use this function to find the residue that is closest to each ivermectin molecule.