Challenge 1

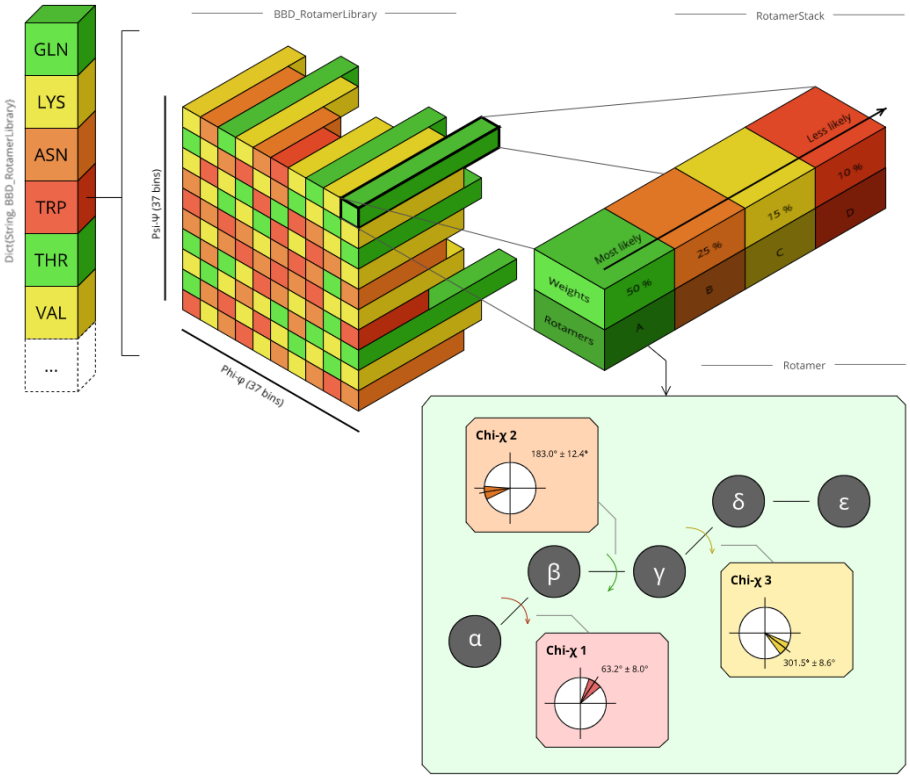
Ex.1) Read and load the Dunbrack rotamer library (which can be found at /class1/dunbrack_rotamers.lib) in such a way that any of the rotamers can be applied to a Molecule (changing the dihedral angles of all *chi* angles). A suggestion is to follow the following schematics:

1.1) A dictionary holds RotamerLibrary objects for each aminoacid type (as a string).

1.2) A RotamerLibrary should hold RotamerStack objects in a Matrix, indexed by the corresponding phi and psi angles. Therefore, a *get_rotamer_stack* function could return the list of rotamers for a given phi and psi values.

1.3) A RotamerStack holds a list of Rotamer objects, as well as the probability of occurrence of each of them. Therefore, a *sample_rotamer_stack* function could return a random Rotamer object, sampled based on the observed weights.

1.4) A Rotamer holds all the chi mean values and corresponding standard deviations. A function *apply_to* could therefore receive a list of atoms (in order) and apply each of the chi angles to the corresponding dihedral (or a value taken from a natural distribution with the mean and standard deviation).



Note: In "/class1/challenge1.py" you will find a dictionary *aminoacid_sc_heavy_atoms* containing all heavy atoms of the sidechain of each aminoacid type. These correspond to the third atom of each *chi-N* dihedral angle of the sidechain.

Ex.2) Sample a rotamer for aminoacid "ARG", based on the measured phi and psi angles of aminoacid 2 on "mol1.pdb" structure. Note that the sampled rotamer should take into account the natural occurrence probability of all rotamers for that specific set of phi and psi angles.

Ex.3) Apply a sampled rotamer (from ex.2) to the aminoacid 2 on "mol1.pdb". Export the changed structure to "mol2.pdb" and observe the changes on PyMOL.

Ex.4) For all aminoacids of "mol1.pdb" structure, sample a new rotamer based on the measured phi and psi angles (taking the natural occurrence probability into account) and apply them to the corresponding aminoacid. Export the changed structure to "mol2.pdb". Perform this loop 10 times, appending a new frame to the "mol2.pdb" trajectory. Observe the results on PyMOL.

Note: When looping over the structure aminoacids, ignore "PRO" and any aminoacid not on the rotamer library (if existent).

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