p(r) bias Guide:

Installation:

1. replace collective variables package with colvars from pr_bias folder (used lammps 2016 originally)
2. go to colvars folder, make colvars package ("make –f Makefile.g++")
3. go to lammps directory make lammps ("make clean-all; make openmpi")

Starting a project:

1. Set up AWSEM
2. Get p(r) from experiment.
3. Normalize to N(N-1)/2. May want to make less bins to speed simulation. Can be done by: "python pr_normalize.py old_file new_file N"
4. Set up collective variables. "python pr_setup.py pdbid", takes p(r) file called $pdbid.pr and makes a new collective variable file called $pdbid.colvars. Also makes a file called alpha.txt which is a vector of 0s to start as alpha.
5. Collective variables options:
    a. PrFile- p(r) file.
    b. alpha- file with a list of numbers with the same length as the number of p(r) bins. Each alpha is the linear bias for that bin.
    c. prindex- each collective variable is a different bin in the p(r). This is the index related to that bin.
    d. cutoff- number of nearest neighbors to exclude, including yourself. Would need to separately remove secondary structure interactions from experimental p(r). Default value is 1.
6. May want to implement a "wall", see example in wall_option. Biases to prevent protein from expanding beyond the maximum size. Must replace max in wall.pr with the maximum protein size.

Proceeding to next iteration:

1. Run LAMMPS simulation
2. If using tempering, create the trajectory at the desired temperature using select_colvars_traj.py
3. If using multiple replicas, combine with combine_colvars.py
4. Calculate Error using calc_error.py. Calculates error, which is the first line of the file. Standard deviation of each histogram bin is subsequent lines. ("python calc_error.py colvars_file pr_file")
5. Calculate next alpha using iterate_alpha.py. ("python iterate_alpha.py old_alpha_file colvars_file pr_file temp tol cutEig force_const"). Reasonable values for the force_const are 0.005-0.0001. Often, it is helpful to try a few values of the force constant at the same time to speed up convergence.
6. Result is a file called new_alpha.txt. Replace alpha.txt with this file and repeat the LAMMPS simulation until error has converged, approximately 10-5%.