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Ch121A Summary
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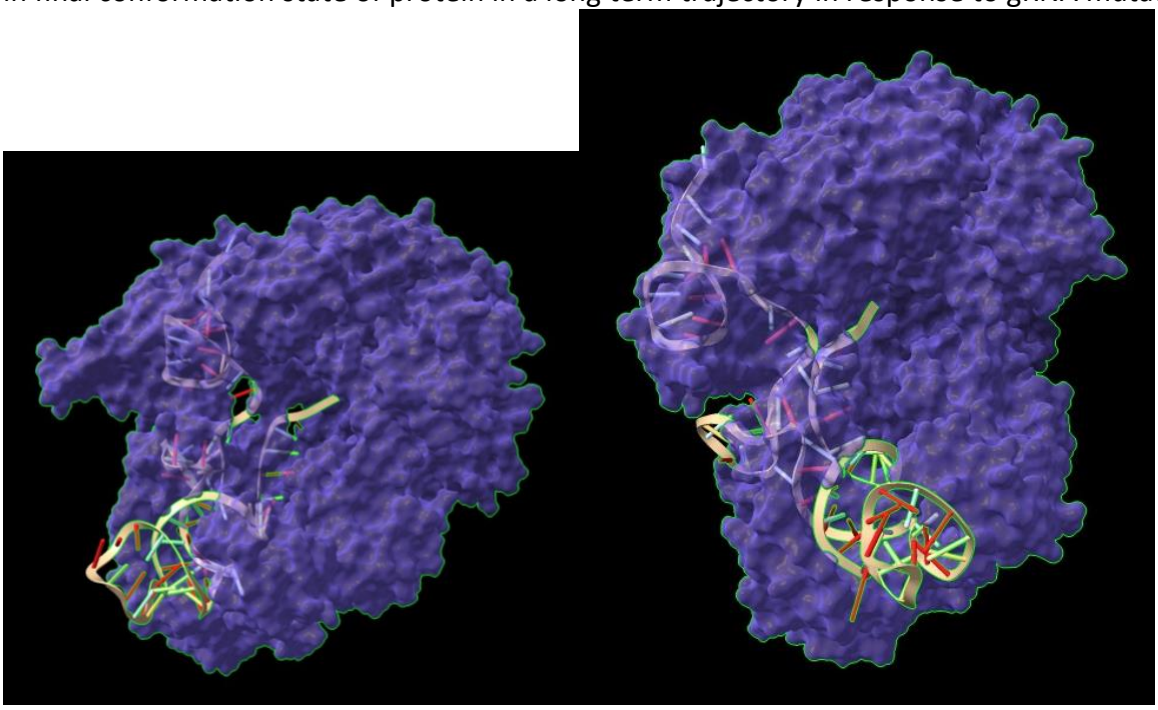
Approach
Look at two different conformations of gRNA bound to Cas9 as starting point for meta-dynamics simulation. Begin by relaxing structures first and then modifying gRNA structures to see if there are any important nucleotide base pair or residue interactions.

Model system:
The initial model system how dCas9 loading the gRNA. I want to see if there are any differences in final conformation state of protein in a long term trajectory in response to gRNA mutations.


Two different views of system 1

RNA = 2317 atoms
dCas9 = 22453 atoms
RNA + dCas9 = 24770 atoms

The total number of atoms of just protein seem ok. Amir advised then system should be less than 200e3 atoms. Given this constraint, the number of total molecules of water which can be added is 58410 or 175230 water atoms.

A [12 12 12] spc216 water box is 173181 water atoms, which satisfies this constraint. I am not sure of the box maybe too small.

I am waiting and trying to interpret the results of initial relaxation experiment.