This MD\_simuations & MD\_simuations\_scripts directory contains the simulation trajectories for the Tead4 double motif bound to two Tead4 proteins.

Following are the simulation folder files that can be accessed upon request sent to email libraryservices@stowers.org.

1. tjp1\_wild\_type
2. tjp1\_left\_side\_mut
3. tjp1\_right\_side\_mut
4. tjp1\_1bp\_insertion\_mut
5. tjp1\_1bp\_deletion\_mut
6. amotl2\_wild\_type\_low\_affinity

Each of the above folder files consists of:

\* notes.txt gives the sequence that was used to build the simulation system, and any other remarks.

\* comb.inpcrd, comb.pdb, and comb.prmtop give the initial configuration of the whole (hydrated) system. This is the starting point of our simulations.

\* deh.inpcrd, deh.prmtop, and deh.dcd give the dehydrated trajectory. deh.inpcrd is at the start of the simulation, and deh.dcd covers the production run.

\* ends.col is the colvar definition file, used to restrain the ends of the DNA and prevent fraying.

\* makeStructure.leap is the file used by tleap (in the AmberTools package) to build the structure.

\* all .namd files give the simulation parameters used for minimization, thermalization, equilibration, and production.

The original, fully-hydrated trajectory files are archived at Stowers and are available upon request.

The scripts directory contains several analysis scripts that were used to generate plots for the publication.

The wild\_type directory additionally contains the protein PDB (5GZB) structure and an example of the B-form DNA generated by Avogadro that was used to build the simulation systems.