1 Usage of protein-DNA modeling

The "proteins.dat" file contains the protein parameters for the "wlmc-standalone-cyclization" application. The input is PDB formatted structures and base-pair step parameters. Output of DNA chains is in X3DNA format (3DNA code by Xiang-Jun Lu, Wilma Olson laboratory - use "rebuild -atomic" option with standard BDNA parameters for the backbone to convert step parameters to all-atom models) and positioned proteins on the loops as PDB files. Any molecular visualization code can be used to visualize the resulting PDB output files (atomic-level DNA and atomic-level protein PDB files).

2 Usage of DNA and ion electrostatics

Two program codes "wlmc-screened" and "mcion" implement different levels of modeling for dsDNA and other macromolecules and their interactions with ions. For coarse-grained DNA phosphate interactions with point ions the "wlmc-screened" can solve the DNA condensation problem with multiple random walkers across several nodes through a client/server framework (hostname and port of the server). The server collects and merges the histograms and outputs the $U * (x)$ (or -PMF(x)) for the system. A few examples of calculating the PMF with radius of gyration is included in the "input.dat" folders, and a DNA sequence is needed to create the DNA, or a PDB file of a macromolecule. The PQR format uses the additional columns of PDB file for the charge and radius of the atoms.