AdKGromacsTutorial Documentation

Release 1.1

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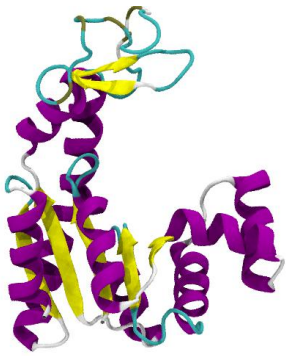

CHAPTER 1

Objective

Perform an all-atom molecular dynamics (MD) simulation—using the Gromacs MD package—of the apo enzyme adenylate kinase (AdK) in its open conformation in a physiologically realistic environment, and carry out a basic analysis of its structural properties in equilibrium.

CHAPTER 2

Tutorial files

All of the necessary tutorial files can be found on GitHub and can be obtained by cloning the repository:

```
git clone https://github.com/Becksteinlab/AdKGromacsTutorial.git
```

CHAPTER 3

Workflow overview

For this tutorial we'll use Gromacs (version 5.1.3) to set up the system, run the simulation, and perform analysis. An initial structure is provided, which can be found in the `tutorial/templates` directory, as well as the MDP files that are necessary for input to Gromacs. The overall workflow consists of the following steps: