foldamers Documentation

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CONTENTS

This documentation is generated automatically using Sphinx, which reads all docstring-formatted comments from Python functions in the 'foldamers' repository. (See foldamers/doc for Sphinx source files.)

COARSE GRAINED MODEL UTILITIES

This page details the functions and classes in src/cg_model/cgmodel.py

1.1 'cgmodel' class for OpenMM simulation

Shown below is a detailed description of the 'cgmodel' class object, which contains all information about a coarse grained model.

1.2 Other coarse grained model utilities

COARSE GRAINED MODEL PARAMETER ANALYSIS UTILITIES

This page details the modules, functions, and classes in src/parameter_analysis

2.1 Parameter sampling protocols

THERMODYNAMIC ANALYSIS TOOLS FOR COARSE GRAINED MODELING

This page details the functions and classes in src/thermo

3.1 Heat capacity example with pymbar

Shown below are functions/tools used in order to calculate the heat capacity with pymbar.

UTILITIES FOR THE 'FOLDAMERS' PACKAGE

This page details the functions and classes in src/util.

4.1 Input/Output options (src/utilities/iotools.py)

Shown below is a detailed description of the input/output options for the foldamers package.

4.2 Utilities and random functions (src/utilities/util.py)

INDICES AND TABLES

- genindex
- modindex
- search