

A

topology: sys.prmtop
positions: sys.crd

B

project_name: sys
outputpath: output
report: True
report_every: 1000
trajectory: DCD
trajectory_every: 2000
trajectory_new_every: 1e6
restart: rs
restart_every: 1e6
save_state_at_end: True

C

platform: CUDA
platform_properties:
Precision: mixed

D

integrator: LangevinIntegrator
temperature: 300
friction: 0.1
timestep: 1.0
barostat: True
pressure: 1.01325
barostat_interval: 100
minimization_max_iterations: 1000

E

nonbondedMethod: PME
nonbondedCutoff: 1.0 # nm
ewaldErrorTolerance: 0.0005
constraints: HBonds
rigidWater: True

F

stages:

- name: solvent_relaxation
temperature: 300
constrained_atoms: not solvent
minimization: True
steps: 100000
trajectory: DCD
trajectory_every: 1000
- name: production
temperature: 300
minimization: False
steps: 25e6
trajectory: DCD
trajectory_every: 2000