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
```