

System

different topologies,
initial coordinates,
constraint and FEP
tag files

Complex

Ligand

Thermodynamic State

$\lambda = 0.0$

$\lambda = \lambda + \Delta$

$\lambda = 1.0$

$\lambda = 0.0$

$\lambda = \lambda + \Delta$

$\lambda = 1.0$

Replica

different initial velocities

r_1

r_2

r_5

r_1

r_2

r_5

r_1

r_2

r_5

r_1

r_2

r_5

r_1

r_2

r_5

r_1

r_2

r_5