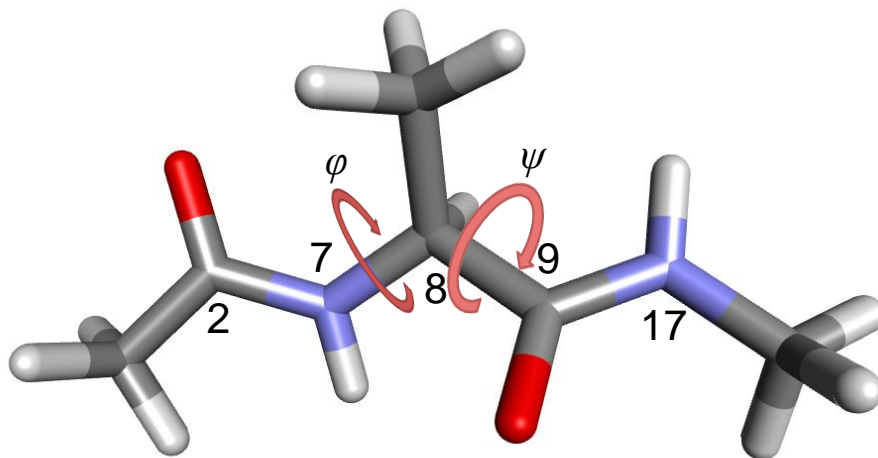


# LogMFD (AFED)

## 1. Calculation setup

The following setup is used.

- Method : AFED
- System : alanine dipeptide
- Number of replica : 8
- AFED Type : NVT
- Collective variables (CV) :
  - cv1 : dihedral angle  $\phi$  (2-7-8-9)
  - cv2 : dihedral angle  $\psi$  (7-8-9-17)
- Initial position of CVs :
  - cv1 : -154.00 degree
  - cv2 : 133.65 degree
- Initial velocity of CVs :
  - cv1 : 0.1
  - cv2 : 0.1
- Number of CVs updates : 10000
- Constrained MD
  - Ensemble : NVT
  - time step : 0.5 fs
  - Potential : MM
  - Temperature : 300 K
  - Number of steps : 2000



## 2. Results

As shown below, the cv values and free energy are printed in “afed.out” .

step	st	cv	r-ideal	r-mean	f-energy	-df/dr	dr/dt	h-energy	temp
0	LO	1	-154.000	-153.875	0.003000	0.000062	0.100000	0.001571	300
0	LO	2	133.650	133.873	0.003000	0.000112	0.100000	0.001571	300
1	LO	1	-153.900	-153.686	0.002983	0.000107	0.100000	0.001571	300
1	LO	2	133.750	133.777	0.002983	0.000013	0.100100	0.001571	300
2	LO	1	-153.800	-153.584	0.002971	0.000108	0.100100	0.001571	301
2	LO	2	133.850	134.206	0.002971	0.000177	0.100100	0.001571	301
3	LO	1	-153.700	-153.553	0.002942	0.000074	0.100200	0.001571	301
3	LO	2	133.950	134.163	0.002942	0.000106	0.100200	0.001571	301
4	LO	1	-153.599	-153.623	0.002924	-0.000013	0.100300	0.001571	302
4	LO	2	134.051	134.256	0.002924	0.000104	0.100300	0.001571	302
5	LO	1	-153.499	-153.208	0.002915	0.000144	0.100300	0.001571	302
5	LO	2	134.151	134.265	0.002915	0.000055	0.100400	0.001571	302

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The molecular structures of each step and each replica are printed in “afed.xyz” . X ITER and Y BEAD are representing cv update number and replica number, respectively.

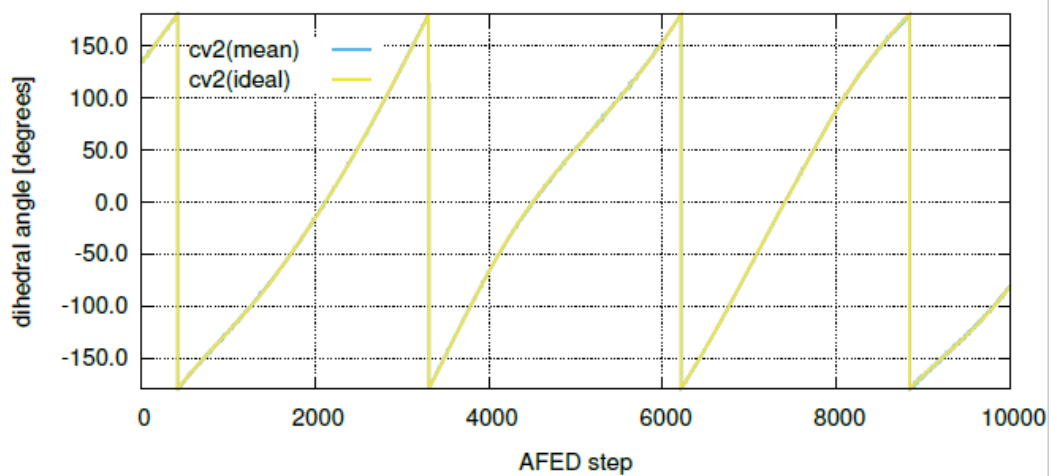
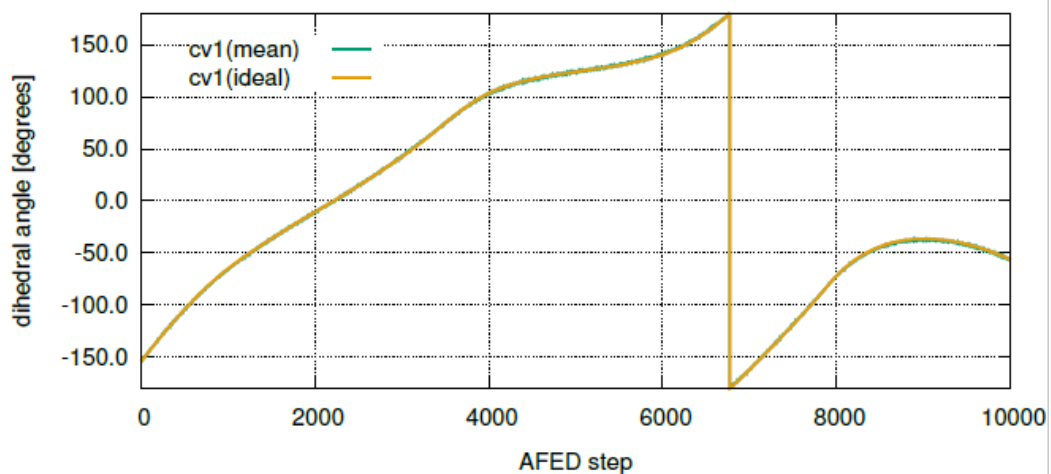
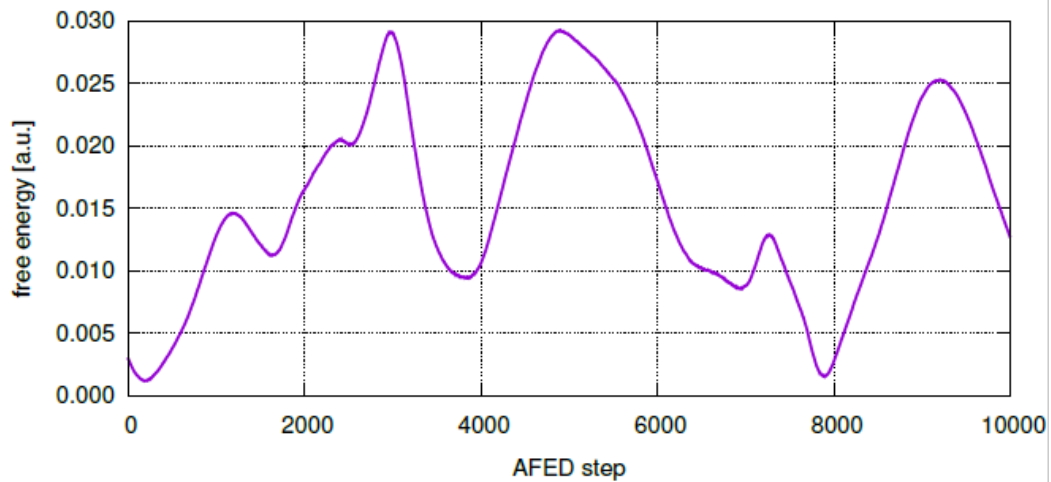
22			
LO	0 ITER	1 BEAD	0.03
CT3	0.14251	5.87000	-6.37483
C	1.39075	5.54128	-7.04126
O	1.52262	4.68107	-7.87827
HA	0.41156	6.60475	-5.55305
HA	-0.57420	6.34822	-7.06042
HA	-0.32026	4.98868	-5.98714
NH1	2.44116	6.24694	-6.63477
CT1	3.76350	6.20651	-7.26309
C	4.72217	6.60865	-6.15125
O	4.39585	7.47273	-5.33645
H	2.32078	6.76028	-5.75100
HB	3.92353	5.15340	-7.57956
CT3	3.76192	7.06066	-8.58569
HA	3.56468	8.17403	-8.50358
HA	4.75924	7.01800	-9.18023
HA	2.99783	6.68519	-9.30272
NH1	5.84176	5.83798	-6.03630
CT3	6.97673	6.15805	-5.28167
H	5.88082	5.02242	-6.61141
HA	7.69642	5.27538	-5.34265
HA	6.67775	6.30142	-4.22289
HA	7.37321	7.12344	-5.65148

22

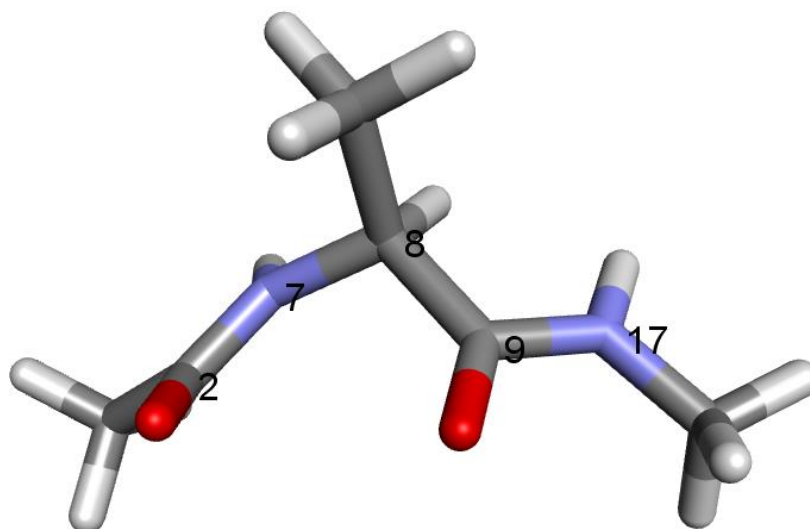
LO	0 ITER	2 BEAD	0.1
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Two cv values and free energies are shown below. Mean cv values change following ideal cv values.



The structure which is the highest free energy is shown below. This structure has most significant contribution of the 8 replicas.



This structure is at the 3000 AFED steps, and the cv values at this time is as shown in the following table.

	ideal	mean
cv1	39.86	39.26
cv2	131.26	131.27

The free energy barrier is estimated to be about 0.0293 hartree.