Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplemental Materials

Computational insights on the destabilization of α-helical conformations formed by leucine zipper peptides in response to temperature

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† X. Xu and X. Xiao have equal contributions to this work.

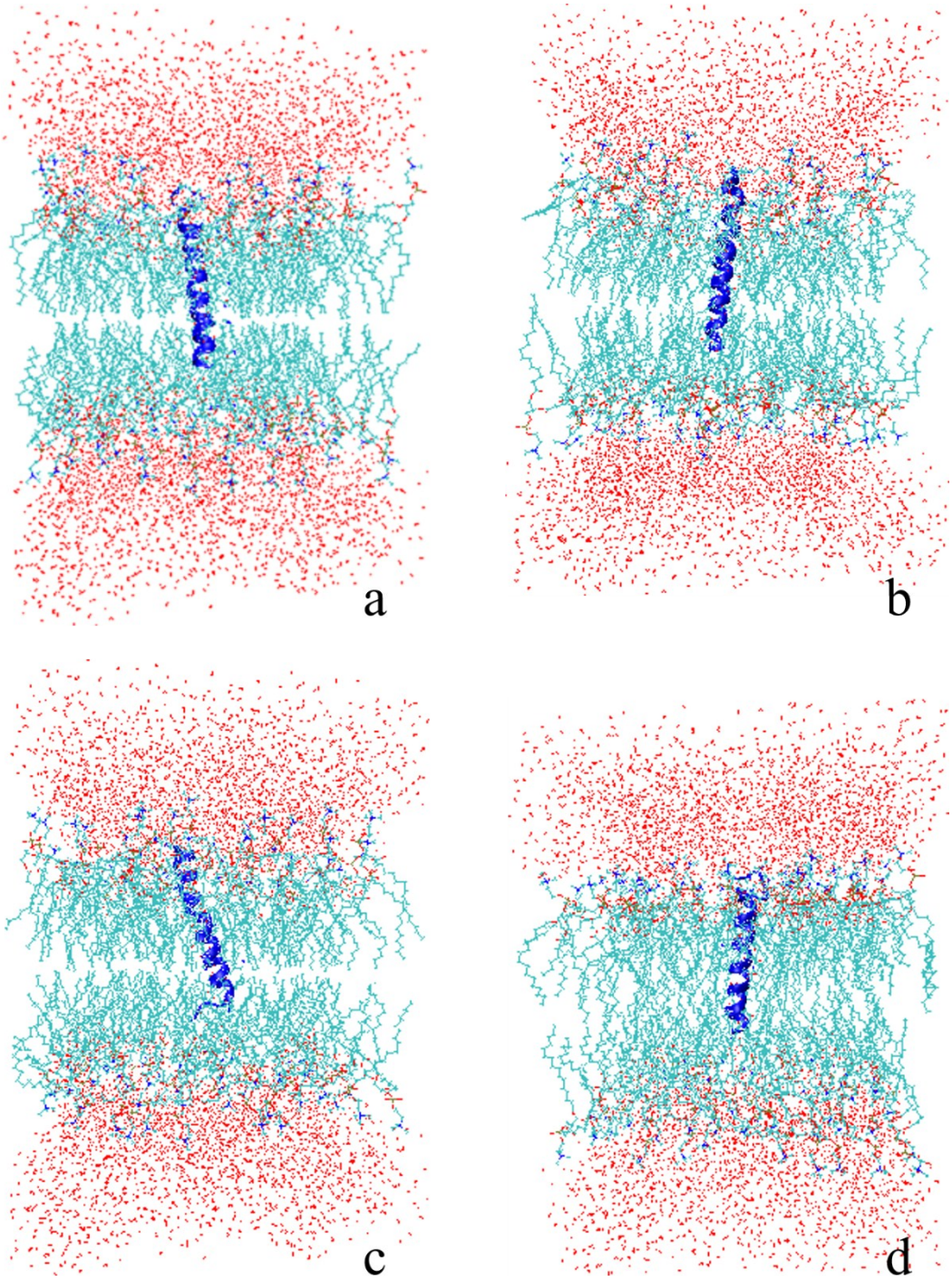


Figure S1. The initial structures of the ALA peptide complexed with lipid DPPC bilayer and water at (a) 315 K, (b) 320 K, (c) 325 K and (d)330 K.

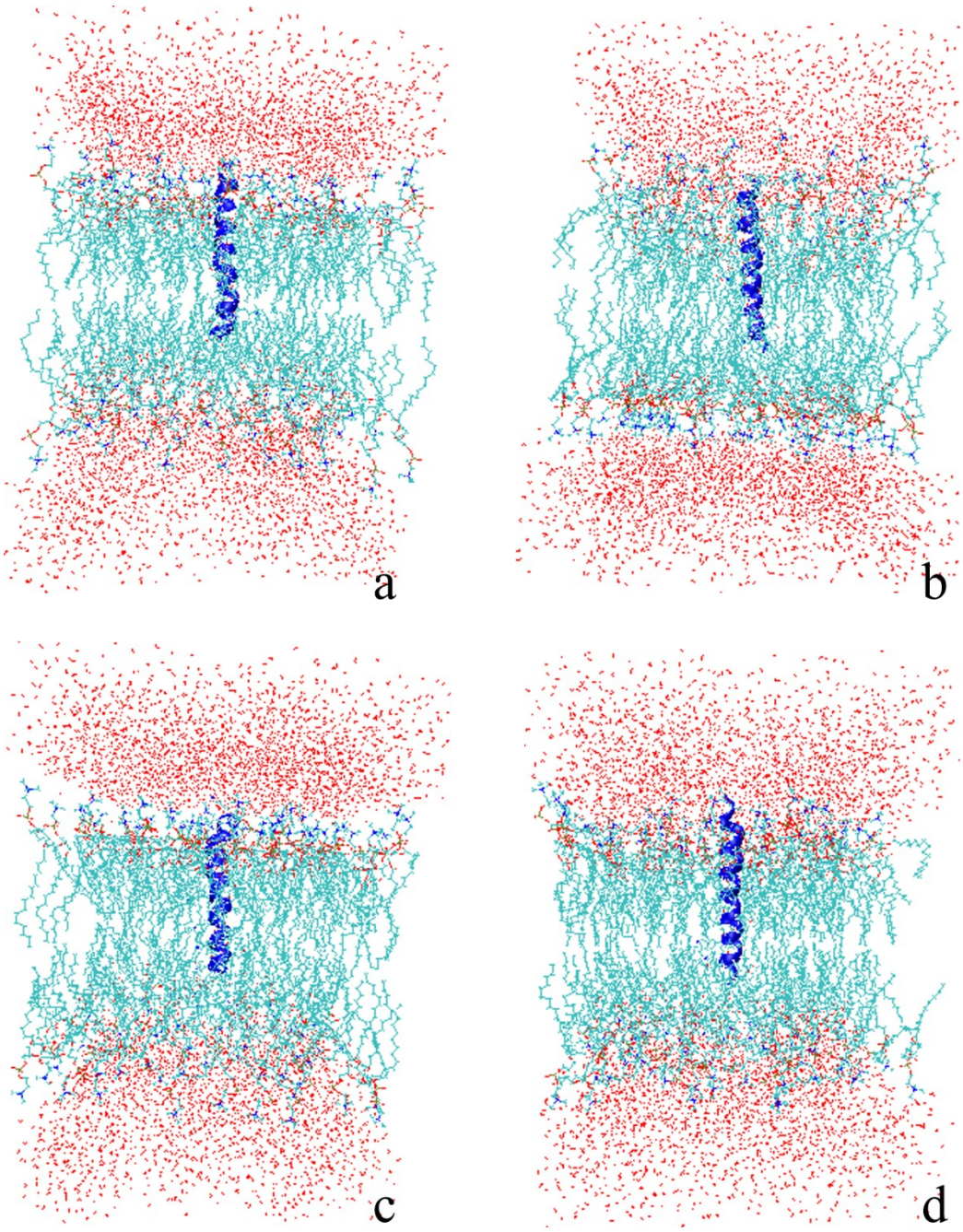
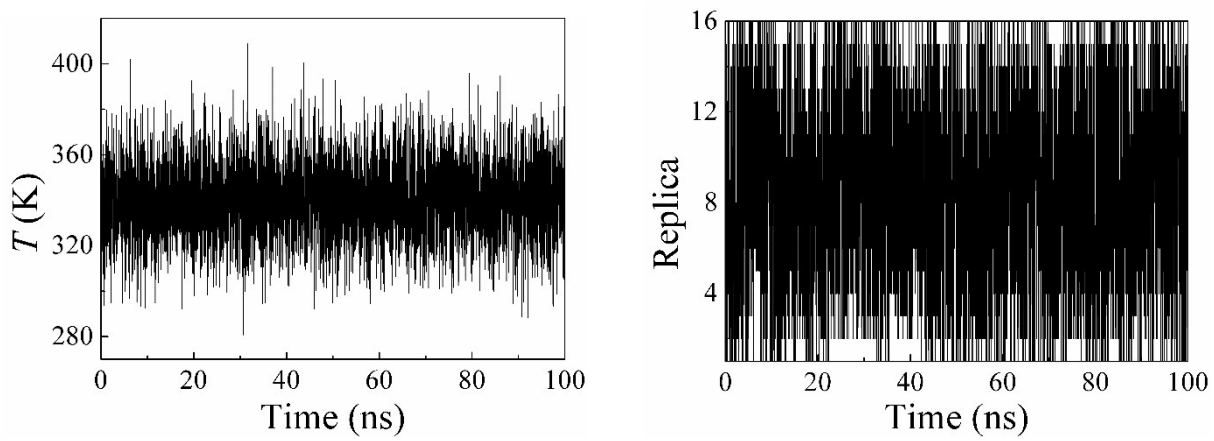
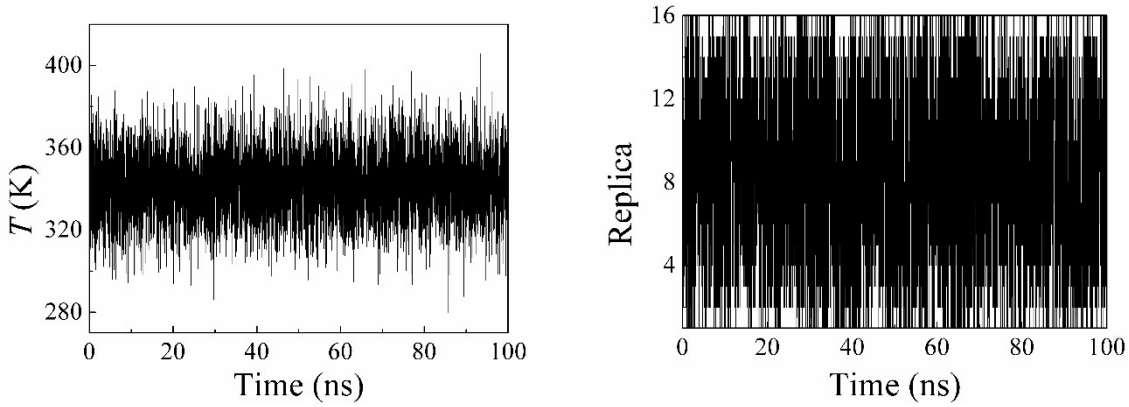


Figure S2. The initial structures of the capped peptide complexed with lipid DPPC bilayer and water at (a) 315 K, (b) 320 K, (c) 325 K and (d)330 K.



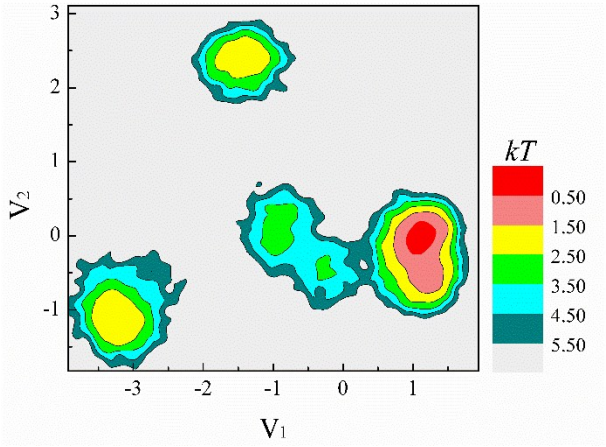
(a) (b)

Figure S3. 100-ns REMD simulation of the ALA peptide. (a) Time series of temperature exchanges for replica 8. (b) Time series of replica exchanges at 325 K.

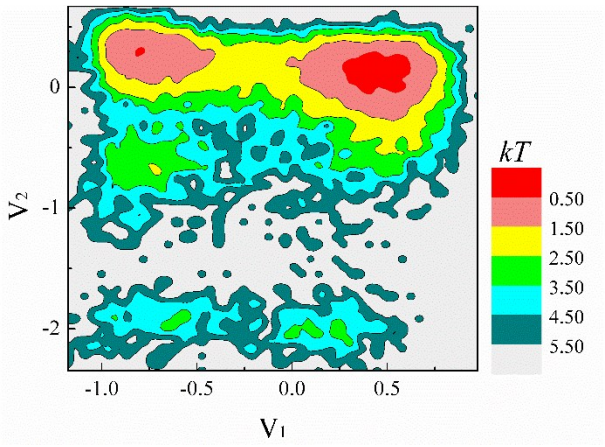


(a) (b)

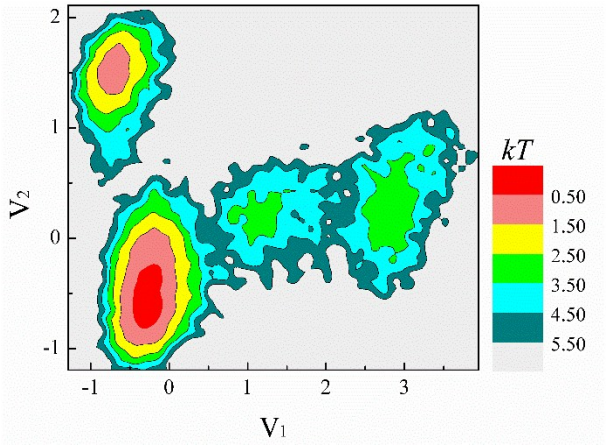
Figure S4. 100-ns REMD simulation of the capped peptide. (a) Time series of temperature exchanges for replica 8. (b) Time series of replica exchanges at 325 K.


kT
0.50
1.50
2.50
3.50
4.50
5.50
V2
V1

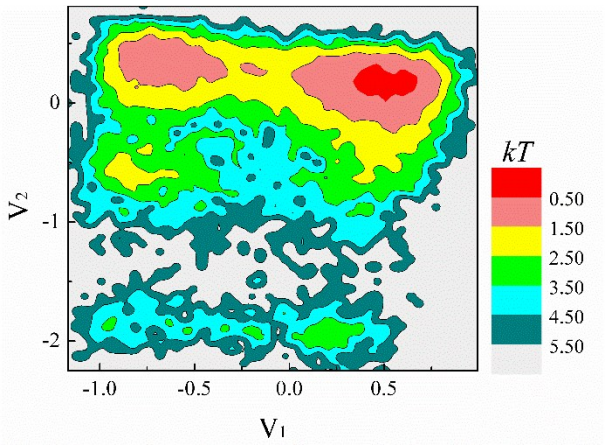
(a)


kT
0.50
1.50
2.50
3.50
4.50
5.50
V2
V1

(b)


kT
0.50
1.50
2.50
3.50
4.50
5.50
V2
V1

(c)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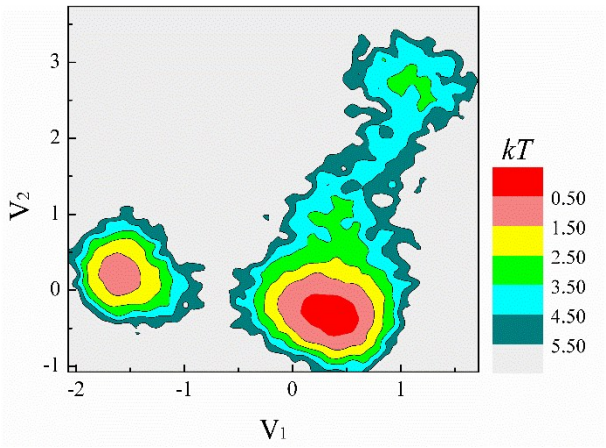
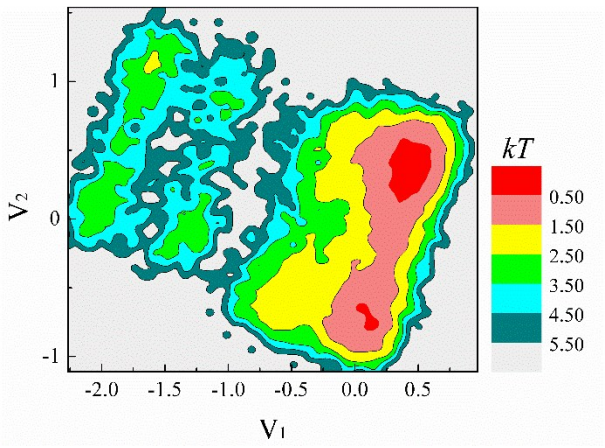
1.50
2.50
3.50
4.50
5.50
V2
V1

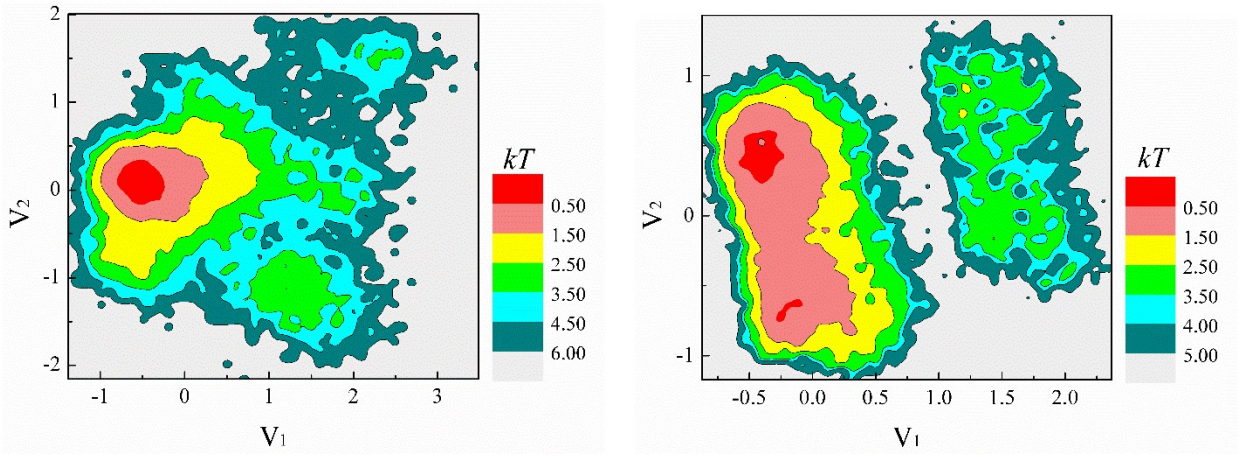
(d)


kT
0.50
1.50
2.50
3.50
4.50
5.50
V2
V1

(e)

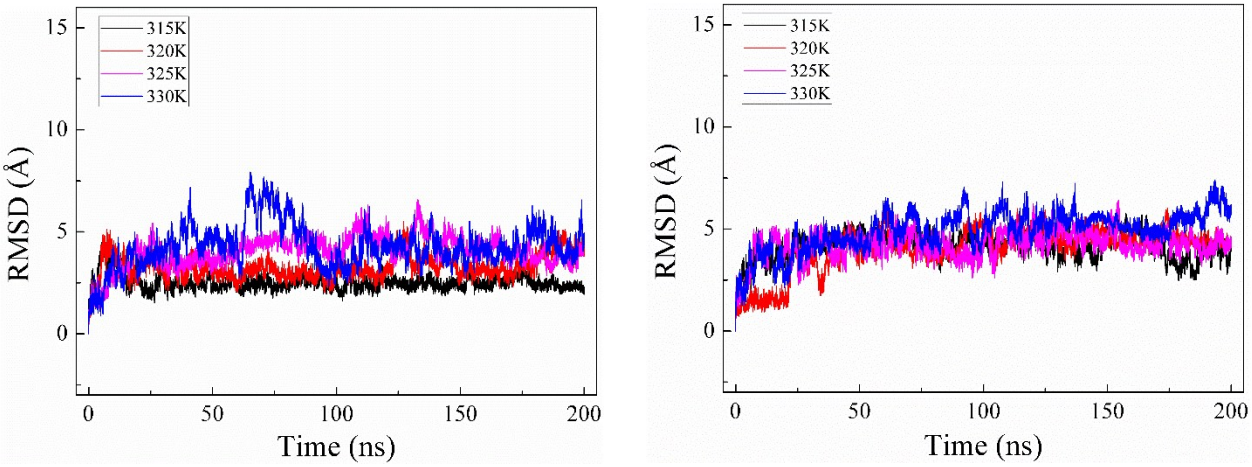

kT
0.50
1.50
2.50
3.50
4.50
5.50
V2
V1

(f)



(g) (h)

Figure S5. Free energy landscape (φ) along the first two principal components (V_1, V_2) for the ALA peptide at (a) 295 K, (c) 320 K, (e) 380 K and (g) 450 K, and for the capped peptide at (b) 295 K, (d) 320 K, (f) 380 K and (h) 450 K.



(a) (b)

Figure S6. The RMSD profiles of the (a) ALA and (b) capped peptides in the 200-ns conventional MD simulations at 315 K, 320 K, 325 K and 330 K