

SUPPLEMENTARY INFORMATION

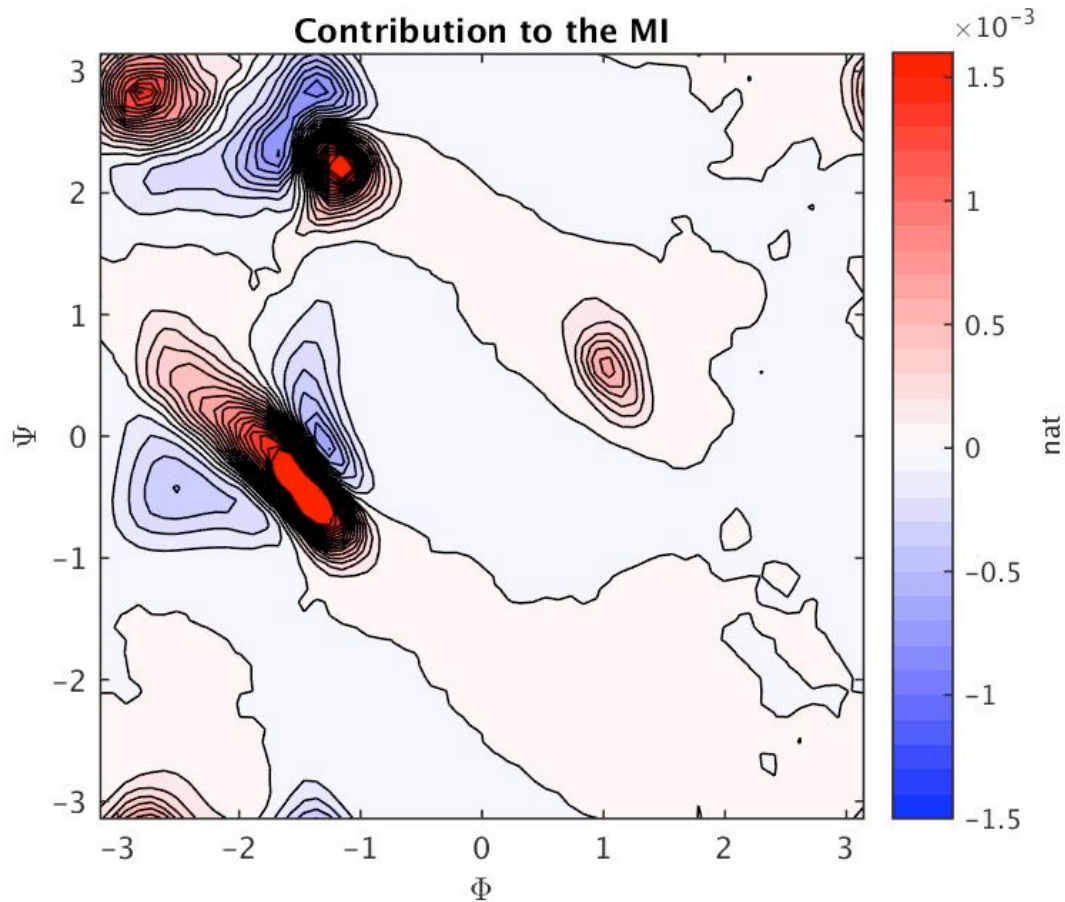


Figure S1: The contribution of each bin of (Φ, Ψ) space to the mutual information. Regions of high thermodynamic coupling do not contribute significantly to the mutual information. Units are shown in nats.

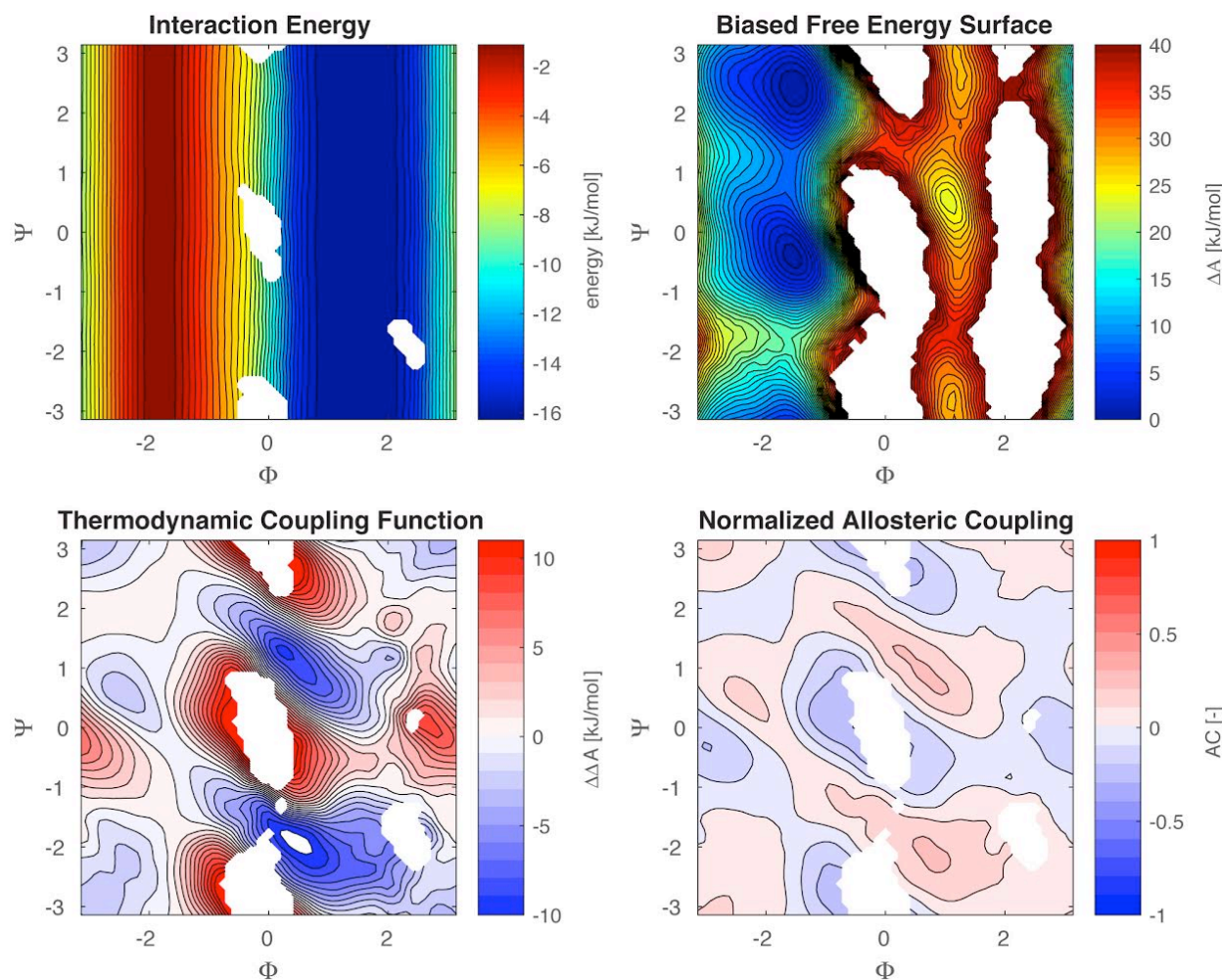


Figure S2: Biasing approach to characterize the contribution of the Φ dihedral energy term to the allosteric coupling function of the alanine dipeptide. (a) Average interaction energy in bins of the (Φ, Ψ) space. (b) The biased free energy surface according to Eq. (28). (c) The biased thermodynamic coupling function, according to Eq. (30). (d) AC corresponding to the biased allosteric function.

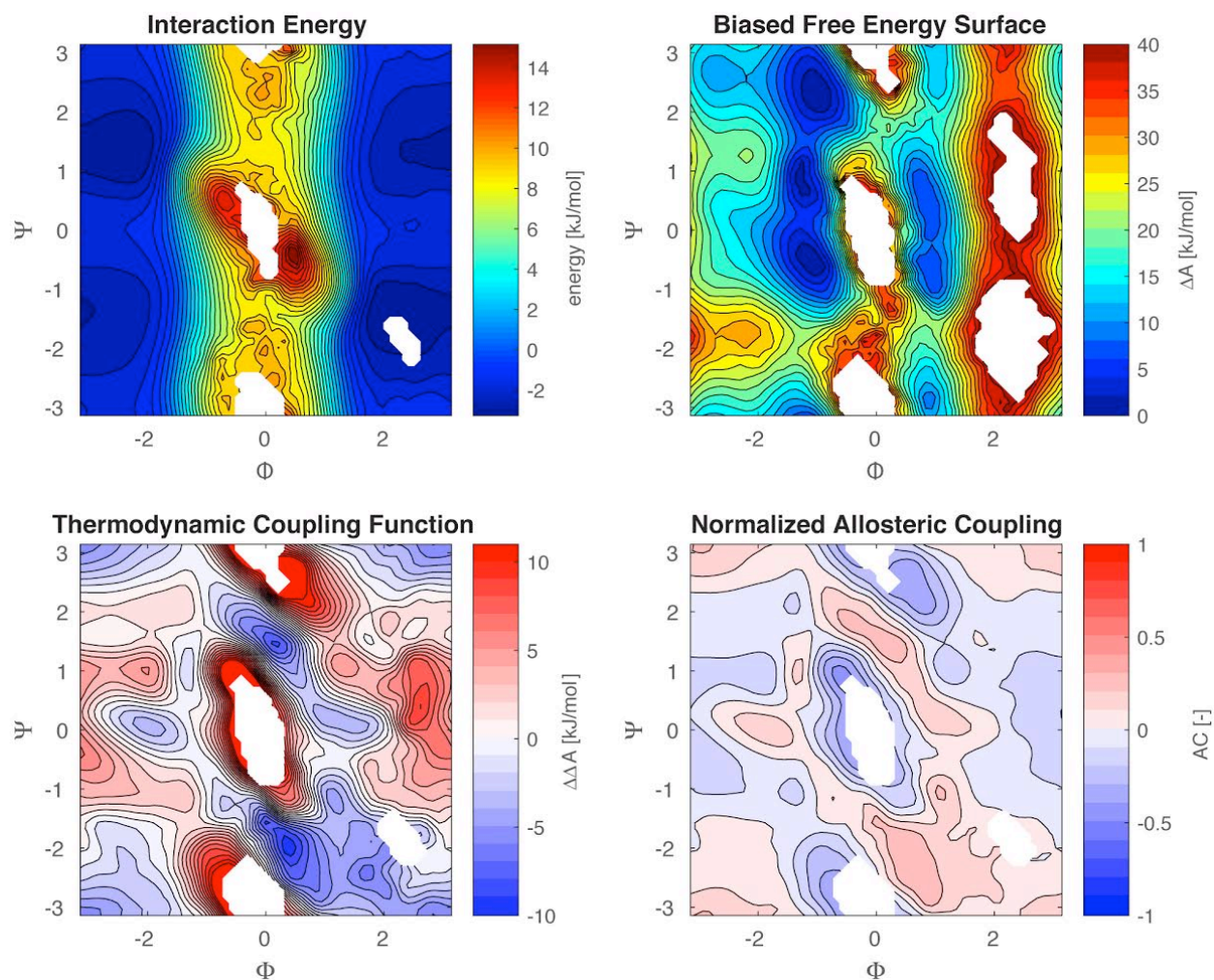


Figure S3: Biasing approach to characterize the contribution of the direct non-bonded interaction energy terms between the N-terminus and the C-terminus of the alanine dipeptide. (a) Average interaction energy in bins of the (Φ, Ψ) space. (b) The biased free energy surface according to Eq. (28). (c) The biased thermodynamic coupling function, according to Eq. (30). (d) AC corresponding to the biased allosteric function.

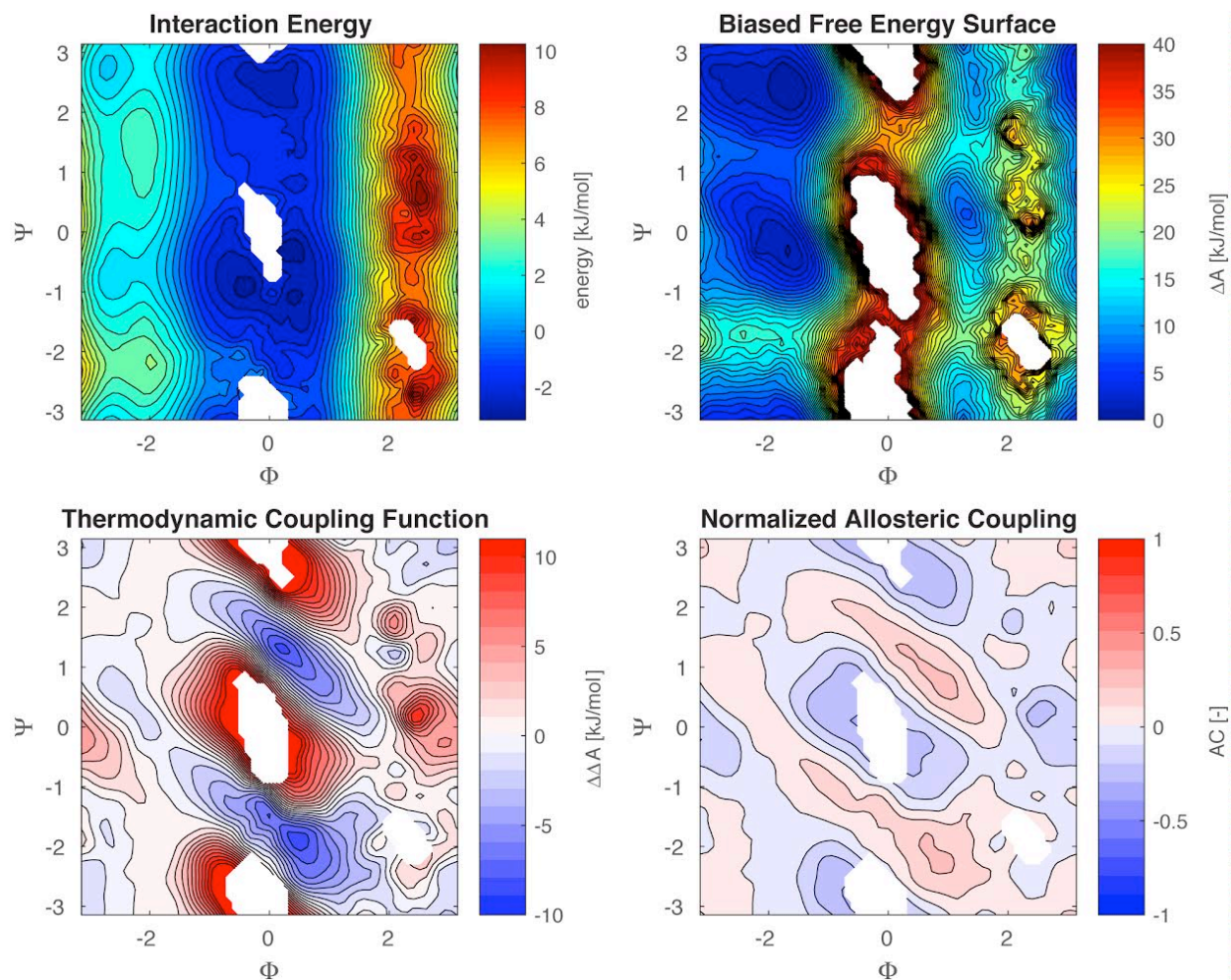


Figure S4: Biasing approach to characterize the contribution of the non-bonded interaction energy terms between the N-terminus and the channel, and between the C-terminus and the channel of the alanine dipeptide. (a) Average interaction energy in bins of the (Φ, Ψ) space. (b) The biased free energy surface according to Eq. (28). (c) The biased thermodynamic coupling function, according to Eq. (30). (d) AC corresponding to the biased allosteric function.

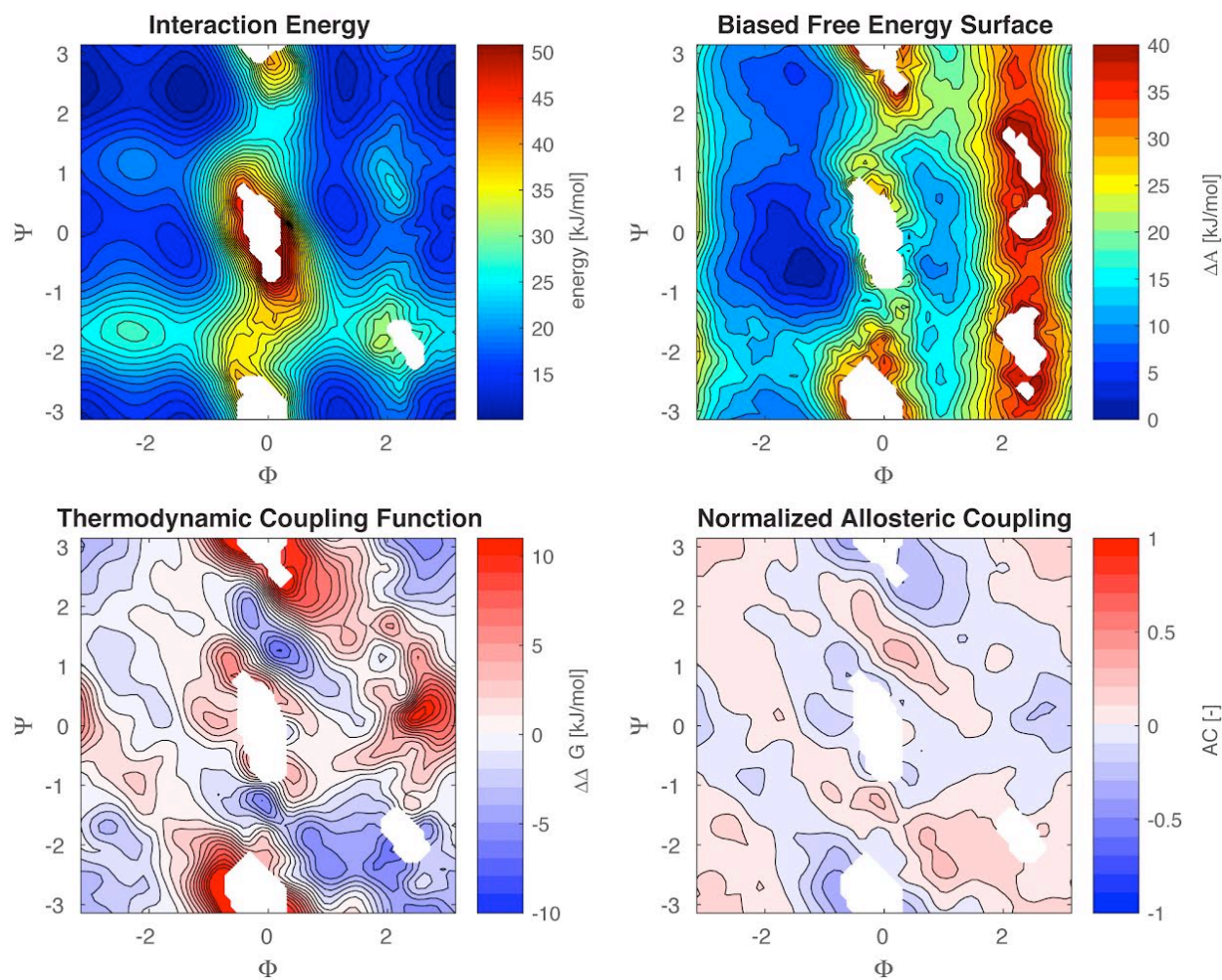


Figure S5: Biasing approach to characterize the contribution of the bonded interaction energy terms involving atoms of the channel and of either the N-terminus or the C-terminus of the alanine dipeptide. (a) Average interaction energy in bins of the (Φ, Ψ) space. (b) The biased free energy surface according to Eq. (28). (c) The biased thermodynamic coupling function, according to Eq. (30). (d) AC corresponding to the biased allosteric function.