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

Supporting Materials

Specific DNA Sequences Allosterically Enhance Protein-Protein Interaction in a Transcription Factor through Modulation of Protein Dynamics: Implications for Specificity of Gene Regulation

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Figure S1. Change in configurational entropy of protein residues of individual subunits of λ-CI due to presence of operator DNA considering all non-hydrogen atoms of the protein residues. (simulation corresponding to ff14SB force field)

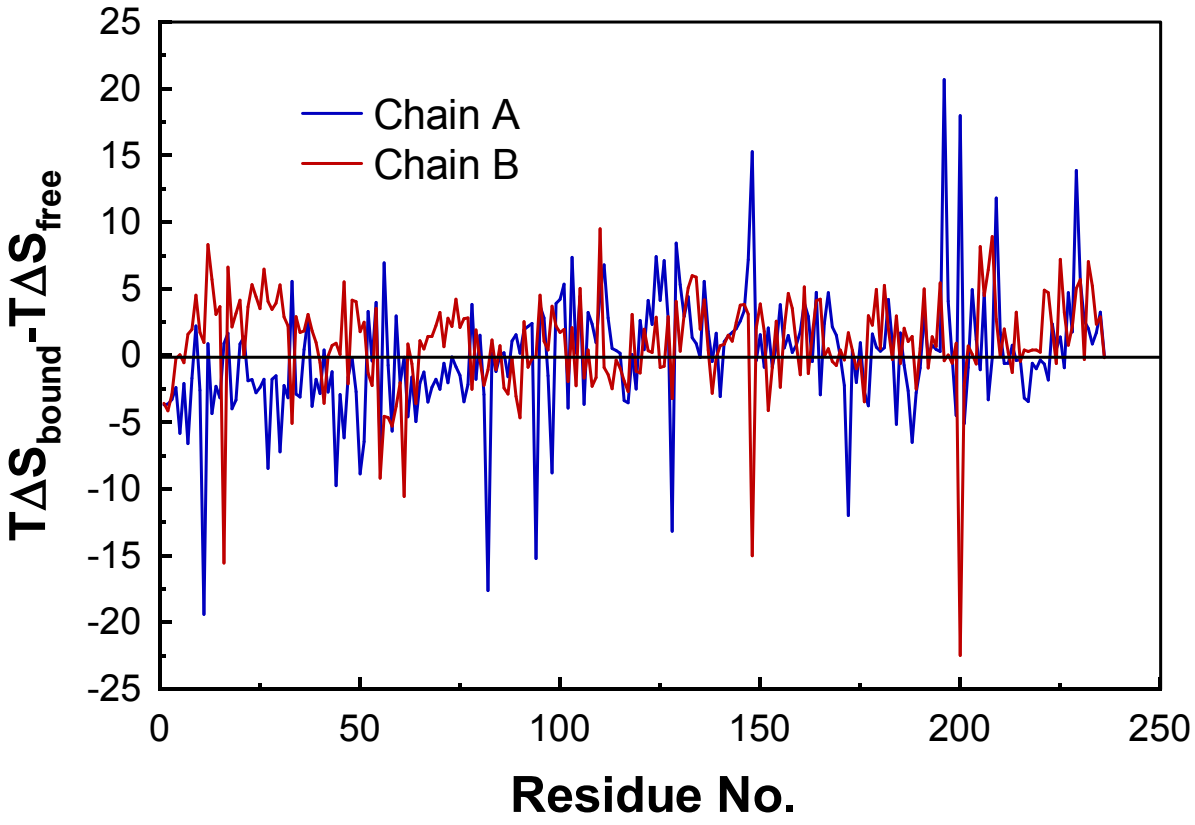


Figure S2. Change in conformational entropy of protein residues of individual subunits of λ-CI due to presence of operator DNA, studied form the distribution of side chain dihedral angle χ1 (simulation corresponding to ff14SB force field).

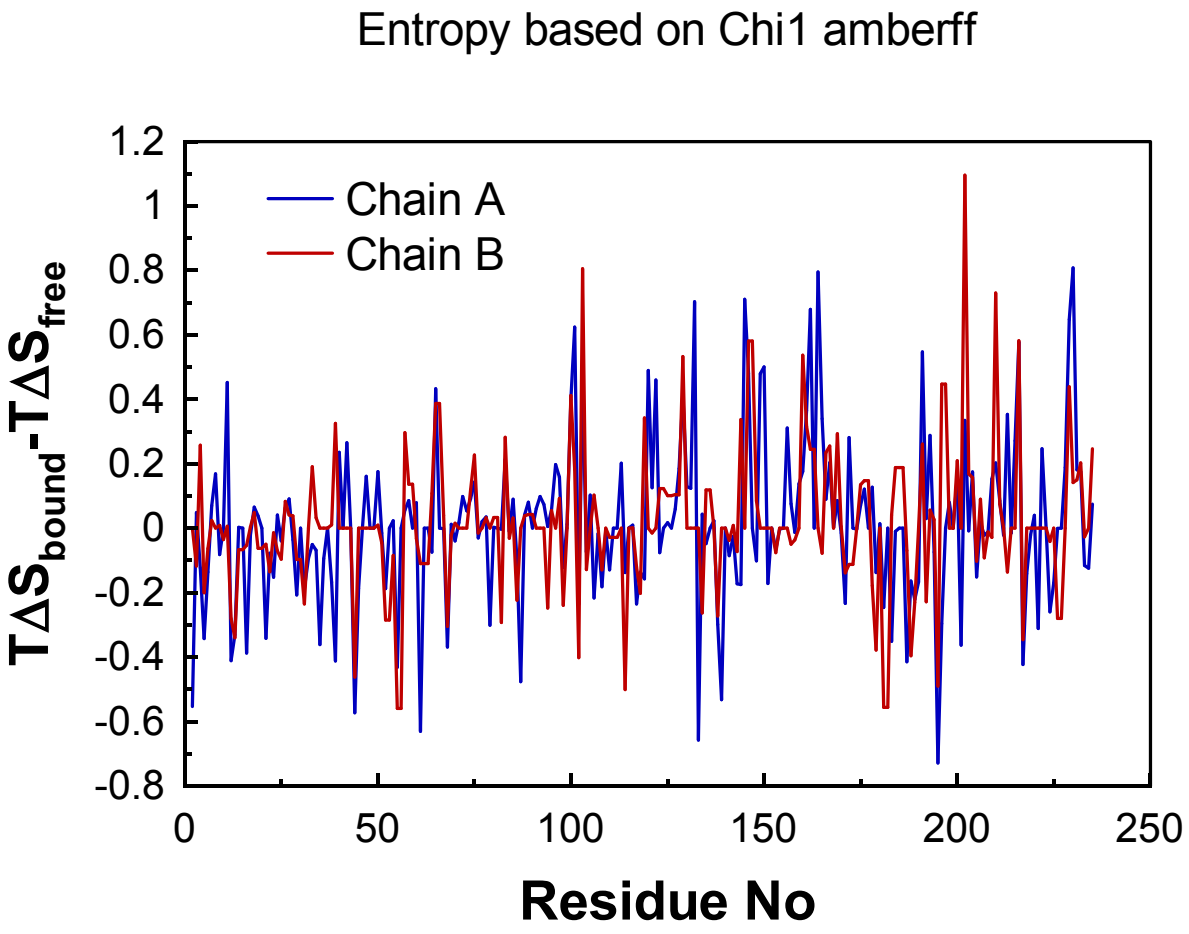


Figure S3: Root mean square fluctuations of residues (considering all non-hydrogen atoms) of the two subunits of λ-CI in the O_L1 bound state (simulation corresponding to parm94 force field).

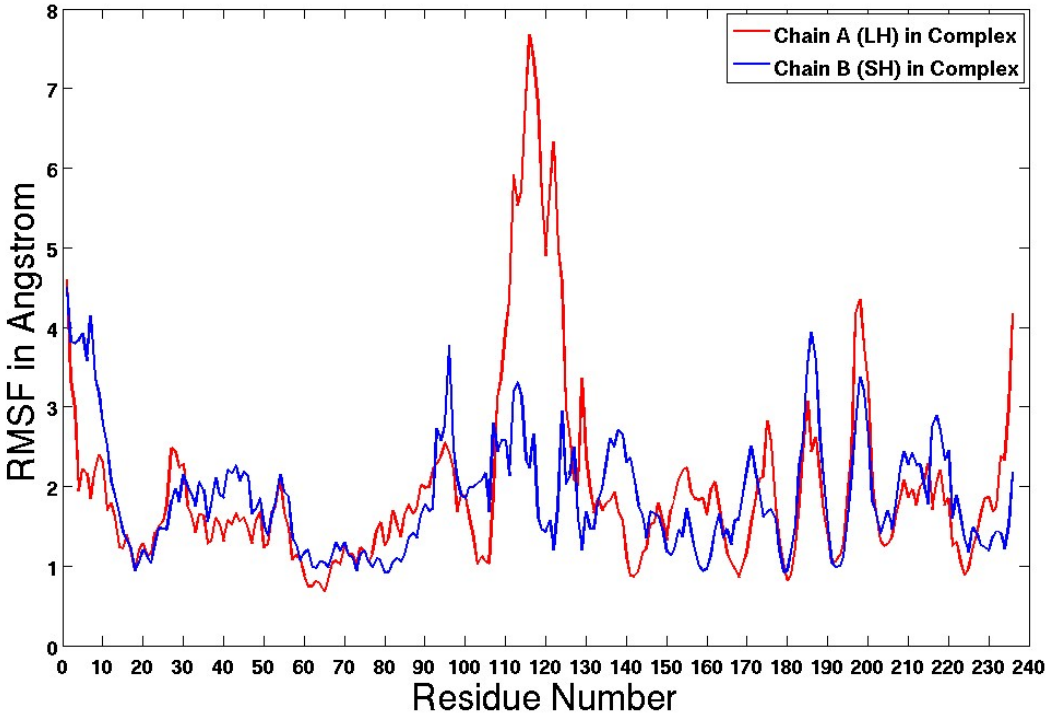
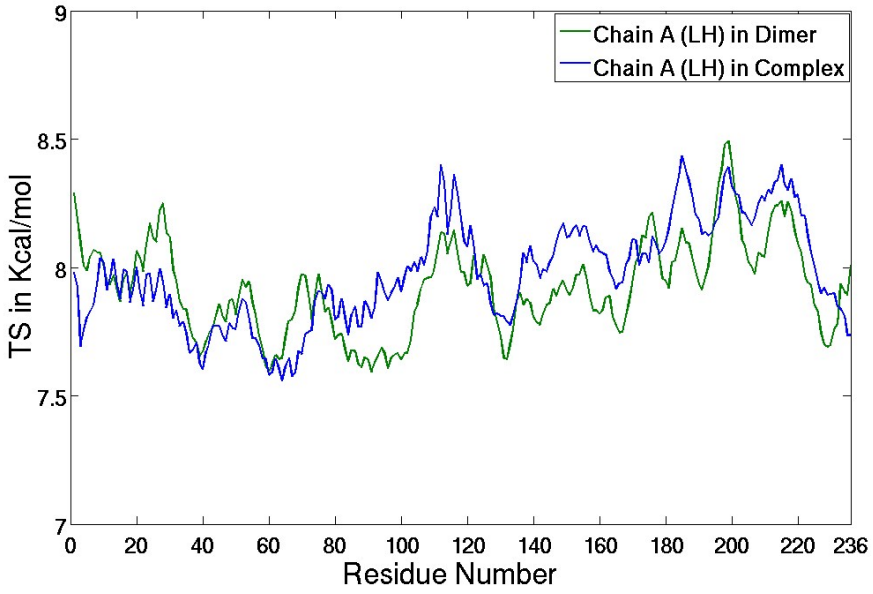
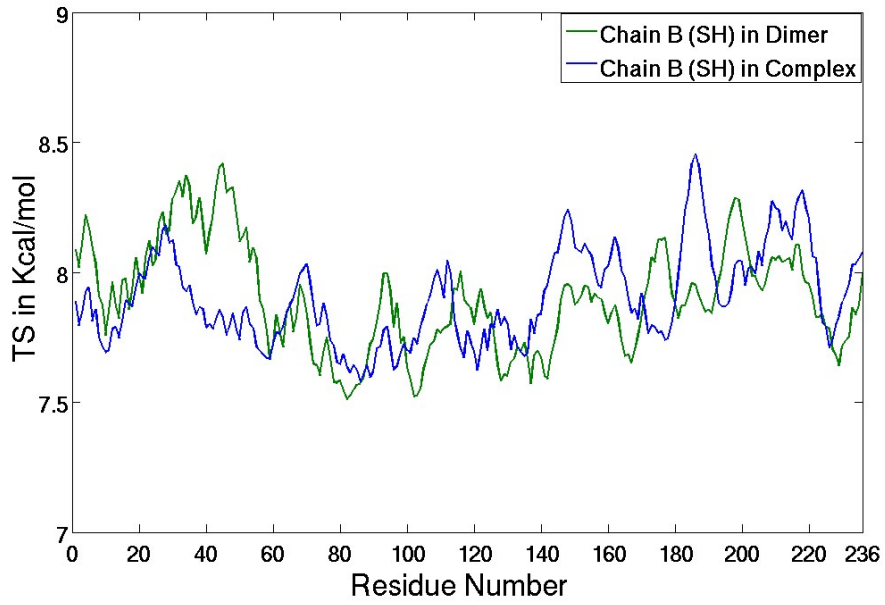


Figure S4: Contribution of Entropy in free energy (TS) of protein residues of the two subunits of λ-CI in the O_L1 bound state and dimeric state. (simulation corresponding to parm94 force field)



(a)



(b)

Figure S5: Ratio of RMSF of Cα atoms and considering side chain atoms of individual subunits of λ-CI in absence and presence of operator DNA for both the chains of λ-CI dimer in operator bound and unbound states were measured (simulation corresponding to parm94 force field).

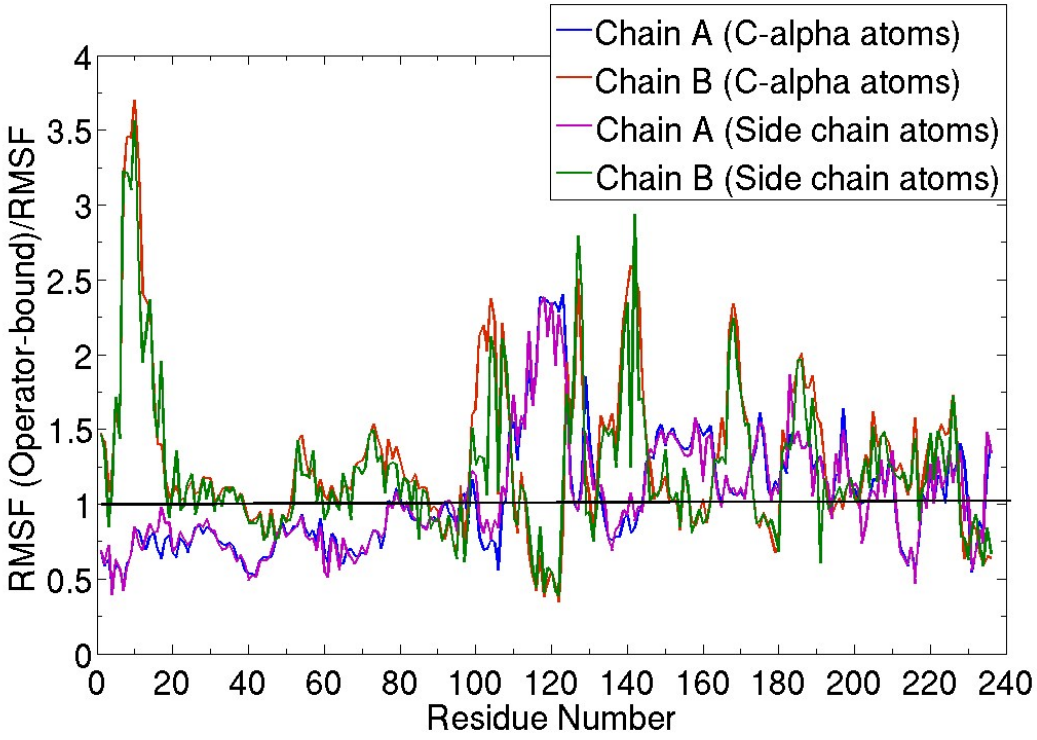


Figure S6: A schematic diagram of alternate geometric arrangements that can lead to protein-protein interaction between two DNA dimers and concomitant DNA loop formation when one protein (in this case, λ–CI) is bound to the same non-target site. The light colored ovals indicate same protein capable of forming different loops.

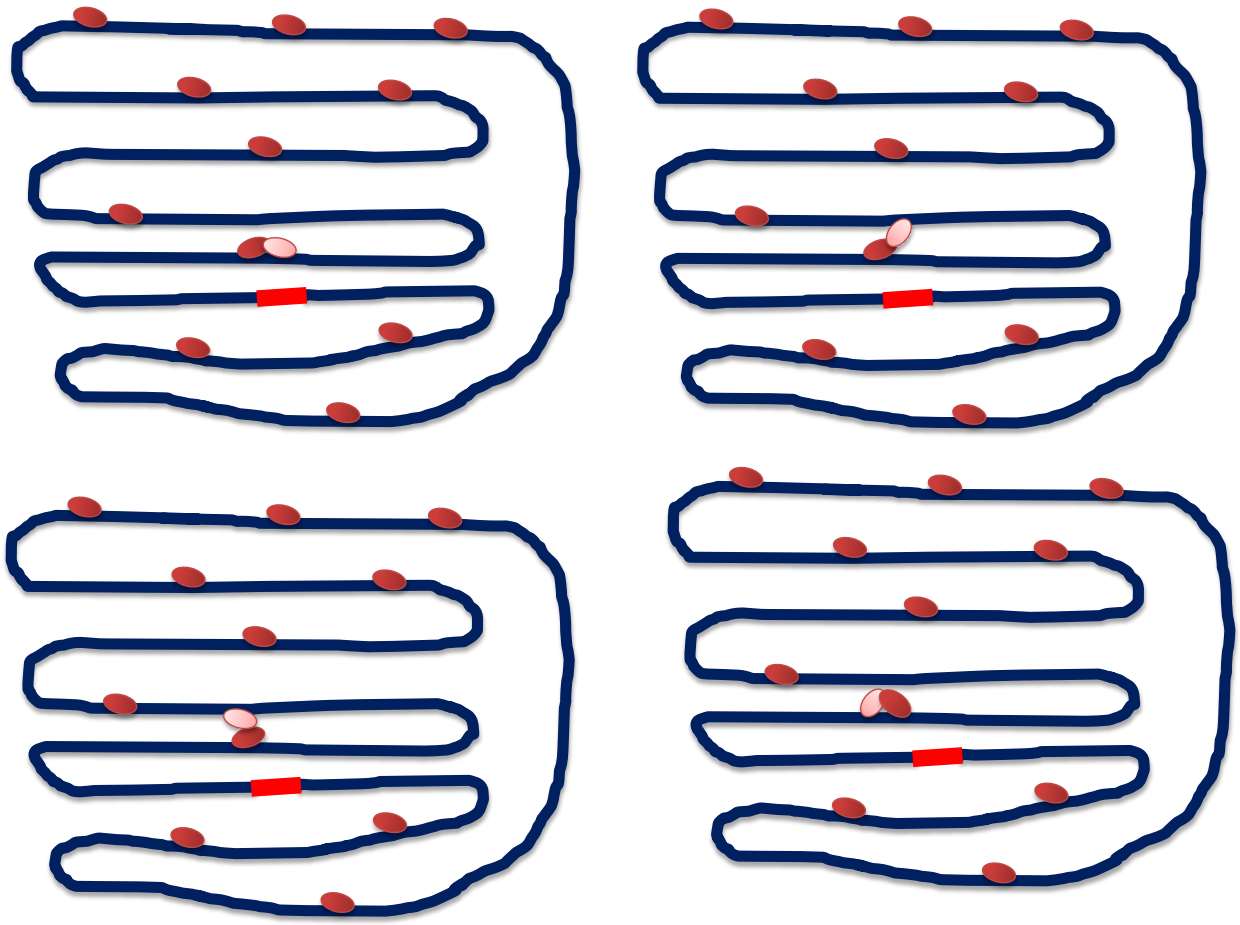


Table S1

Oligo	Sequence
OR1F	5'-CGTACCTCTGGCGGTGATAG-3'
OR1R	5'-CTATCACCGCCAGAGGTACG-3'
OR2F	5'-GCAACACCGTGCGTGTTGTC-3'
OR2R	5'-GACAACACGCACGGTGTTGC-3'

Table S2

Fit of time-resolved fluorescence decay of acrylodan labeled proteins to tri-exponential function

Acrylodan labeled proteins	**τ_1(ns)**	**τ_2 (ns)**	**τ_3 (ns)**	**τ_{avg}**
GC186	0.22±0.03 (23%)	0.84±0.07(56%)	3.37±0.3 (21%)	2.27±0.13
GC186-O_R1	0.18±0.03 (22%)	0.79±0.06 (58%)	3.32±0.2 (20%)	2.20±0.12
GC186-O_R2	0.24±0.05 (24%)	0.78±0.06 (60%)	3.37±0.2 (16%)	2.06±0.14

Table S3

Fit of anisotropy decays to bi-exponential functions

Acrylodan labeled proteins	**τ_{fast} (ns)**	**τ_{slow} (ns)**	**θ (degree)**
GC186CI	0.17±0.02 (15%)	52±2.7 (85%)	18.7±0.3
GC186CI-O_R1	0.12±0.01 (21%)	41±1.5 (79%)	22.5±0.2
GC186CI-O_R2	0.10±0.03 (11%)	53±2.4 (89%)	15.9±0.2