Supplemental Material for Online Publication

for

Cooperative Binding of DNA and CBFβ to the Runt Domain of the CBFα Studied via MD simulations

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Table S1. Simulation systems.

System	Solute Atoms	Added Ions	Total # of Atoms	Box Dimensions
CBFβ-RD-DNA	4621	15(Na^+)	34579	84x64x59
RD-DNA	2581	13(Na^+)	19754	79x57x48
CBFβ-RD	3989	3(Cl^+)	28700	81x67x58
RD	1949	5(Cl^+)	18544	76x57x47
CBFβ	2040	2(Na^+)	14072	65x52x46
DNA1*	632	18(Na^+)	7478	53x41x38
DNA2*	632	18(Na^+)	7478	53x41x38

*Both DNA simulations used the same number of solvent atoms with the DNA1 simulation initiated from the experimental DNA-RD-CBFβ ternary complex structure and the DNA2 simulation initiated from the canonical B-form.

Table S2. RMS difference for backbone atoms of selected CBFβ residues in the vicinity of deleted residues 71 to 79 with respect to the crystallographic coordinates.

Residue	RMS, Å
L66	0.97±0.10
Q67	1.70±0.18
F68	2.45±0.20
F69	4.15±0.17
P70	4.96±0.16
T80	4.66±0.18
P81	1.93±0.06
S82	1.56±0.06
R83	1.00±0.02
E84	1.03±0.03

Table S3. RMS difference of MD simulated structures with X-ray structure 1H9D.

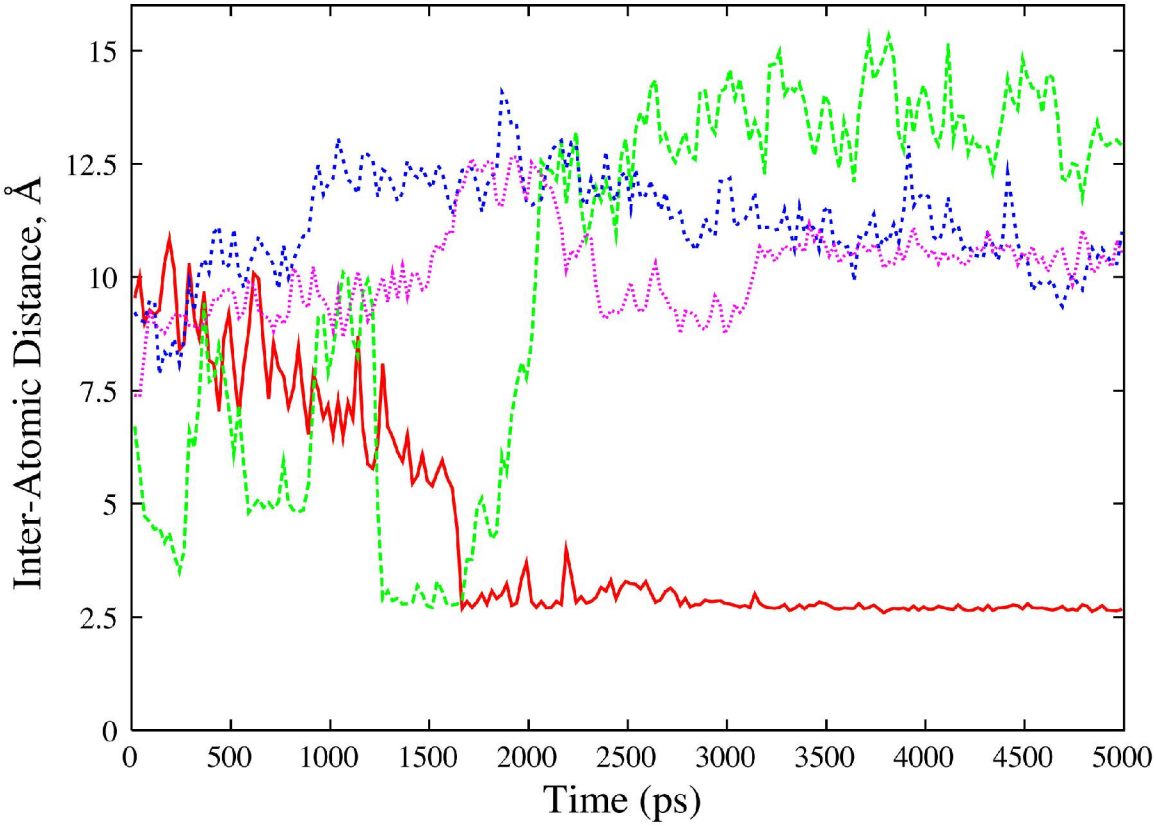
Time, ps	DNA	RD	CBFβ	RD-DNA	RD-CBFβ	CBFβ-RD-DNA
1000	1.53	4.10	2.04	2.46	3.05	2.58
1500	1.45	3.81	2.26	2.71	3.48	2.56
2000	1.65	3.28	2.30	2.97	4.00	2.76
2500	1.55	3.31	2.18	3.63	4.12	2.85
3000	1.62	3.74	1.99	3.09	3.79	2.88
3500	1.57	3.34	2.00	3.21	3.67	2.89
4000	1.89	3.74	2.18	3.54	3.31	2.98
4500	1.55	3.40	2.21	3.84	3.66	2.92
5000	1.73	3.28	2.24	3.65	3.59	2.83
Average	1.62±0.04	3.56±0.10	2.15±0.04	3.23±0.16	3.63±0.11	2.81±0.05

Table S4. Total Energy and Energy Components for the Systems Studied.

System	G[a]	$G_{Solvation}$[b]	E_{strain}[c]	$E_{interaction\ energies}$			Entropy TS[d]
				RD-DNA[e]	RD-CBFβ[f]	CBFβ-DNA	
Trimer	-10683±7	-5675±35	-2132±32	-2623±13	-299±10	45±8	3424±5
RD-DNA	-5719±6	-3951±22	745±15	-2513±12			1933±3
CBFβ-RD	-8118±9	-3561±44	-4319±51		-239±3		2972±5
RD	-3159±3	-1897±20	-1262±18				1477±3
CBFβ	-4877±4	-1925±19	-2952±18				1544±0
DNA1[g]	-2559±1	-4457±4	1898±5				505±0
DNA2[g]	-2558±1	-4461±4	1903±4				

Energies in kcal/mol averaged over the MD simulations with standard errors reported. [a] Total free energy of each system based on equation 2 without entropy contribution; [b] Solvation energy of the system, including electrostatic and non-polar contributions; [c] Strain energy calculated as described in the methods; [d] TS calculated at 300 K. [e] Interaction energy between RD and DNA in the presence and absence of CBFβ; [f] Interaction energy between RD and CBFβ in the presence and absence of DNA. [g] DNA1 and DNA2 represent the simulations initiated from the experimental DNA-RD-CBFβ ternary complex structure and from the canonical B form, respectively.

Figure S1



Distances, in Å, between RD Glu116 and CBFβ Arg33 atoms CA-CA and OE2-NH2 as a function of simulation time. Blue and cyan lines show distances for CA-CA atoms for the RD-CBFβ binary and ternary complexes, respectively, while green and red lines show OE2-NH2 distances for the RD-CBFβ binary and ternary complexes, respectively.