Supporting Information

Molecular Simulations on the Thermal Stabilization of DNA by Hyperthermophilic Chromatin Protein Sac7d, and Associated Conformational Transitions

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Table S1: Average RMSD values (Å) of the DNA molecules calculated for all possible 2, 3, 4 and 5 base pair steps with respect to the X-ray crystal structures.

AZP	360-1	360-2	AZQ	360-1	360-2
2 BASE PAIRS STEPS					
C2G7-G3C6	1.21 ± 0.05	1.48 ± 0.34	**T2A7-A3T6**	2.42 ± 0.17	3.11 ± 0.46
G3C6-A4T5	1.16 ± 0.04	1.19 ± 0.02	**A3T6-A4T5**	1.28 ± 0.08	1.70 ± 0.17
A4T5-T5A4	0.90 ± 0.03	0.88 ± 0.01	**A4T5-T5A4**	1.04 ± 0.07	1.16 ± 0.07
T5A4-C6G3	0.72 ± 0.06	0.78 ± 0.08	**T5A4-T6A3**	1.11 ± 0.06	0.85 ± 0.02
C6G3-G7C2	0.98 ± 0.12	1.41 ± 0.32	**T6A3-A7T2**	1.61 ± 0.17	1.04 ± 0.14
3 BASE PAIR STEPS					
C2G7-A4T5	1.25 ± 0.04	1.54 ± 0.30	**T2A7-A4T5**	2.22 ± 0.13	2.79 ± 0.37
G3C6-T5A4	1.16 ± 0.02	1.16 ± 0.03	**A3T6-T5A4**	1.35 ± 0.03	1.65 ± 0.13
A4T5-C6G3	0.96 ± 0.05	0.96 ± 0.05	**A4T5-T6A3**	1.20 ± 0.07	1.22 ± 0.08
T5A4-G7C2	0.99 ± 0.12	1.32 ± 0.27	**T5A4-A7T2**	1.60 ± 0.13	1.08 ± 0.10
4 BASE PAIR STEPS					
C2G7-T5A4	1.25 ± 0.03	1.50 ± 0.27	**T2A7-T5A4**	2.11 ± 0.11	2.57 ± 0.32
G3C6-C6G3	1.19 ± 0.02	1.18 ± 0.06	**A3T6-T6A3**	1.42 ± 0.00	1.68 ± 0.12
A4T5-G7C2	1.12 ± 0.11	1.36 ± 0.21	**A4T5-A7T2**	1.61 ± 0.13	1.31 ± 0.12
5 BASE PAIR STEPS					
C2G7-C6G3	1.30 ± 0.03	1.52 ± 0.26	**T2A7-T6A3**	2.08 ± 0.09	2.49 ± 0.27
G3C6-G7C2	1.31 ± 0.08	1.46 ± 0.18	**A3T6-A7T2**	1.73 ± 0.08	1.72 ± 0.15

Alignments of the structures from the trajectories on to the X-ray crystal structures were based on the parts of the DNA on which the RMSD values were calculated.

Table S2: Percentage of base pair closed states in the MD simulations on DNA and protein-DNA complexes computed based on N1-N3 distances with a cutoff of 3.5 Å.

	DNA (alone)				DNA (complexed)				
AZP	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
C2-G7	99.9	53.5	33.7	2.2	99.8	99.3	88.3	39.6	2.4
G3-C6	99.9	77.6	38.7	4.5	99.1	99.3	98.4	48.8	11.8
A4-T5	99.8	99.9	37.8	4.2	99.8	99.1	98.9	47.1	10.9
T5-A4	99.8	99.5	32.8	5.1	99.7	99.6	99.7	55.5	5.9
C6-G3	99.9	84.5	32.8	4.1	99.9	99.6	99.8	56.3	10.4
G7-C2	99.9	81.9	25.2	5.4	99.9	98.4	83.4	21.9	5.1
AZQ	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
T2-A7	99.9	1.6	4.8	1.3	99.8	33.6	51.7	2.1	0.9
A3-T6	99.1	27.6	6.1	1.0	99.8	94.6	32.9	7.2	3.6
A4-T5	100.0	45.8	15.9	0.0	99.8	96.4	96.4	5.7	5.7
T5-A4	99.9	45.2	16.1	1.7	99.8	96.5	99.3	8.8	6.8
T6-A3	99.9	42.9	14.8	1.7	99.9	92.5	99.6	10.5	6.1
A7-T2	99.9	32.7	1.8	0.2	99.8	65.5	93.3	8.9	2.9

Table S3: Intra strand stacking interaction energies of the central four base pairs (kcal/mol) of the DNA molecules present in the two binary complexes obtained from different MD simulations.

	DNA (alone)				DNA (complexed)				
AZP	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
1G3	-20.6 ± 0.1	-17.4 ± 1.5	-7.4 ± 3.2	-1.0 ± 0.5	-19.8 ± 0.2	-19.2 ± 0.4	-18.4 ± 1.2	-11.4 ± 2.5	-0.4 ± 0.1
1A4	-17.9 ± 0.1	-16.4 ± 0.5	-5.6 ± 2.9	-0.9 ± 0.4	-16.4 ± 0.1	-16.1 ± 0.1	-16.1 ± 0.1	-11.3 ± 1.7	-0.8 ± 0.4
1T5	-9.4 ± 0.1	-8.7 ± 0.2	-2.4 ± 1.1	-2.2 ± 1.1	-9.0 ± 0.2	-7.5 ± 0.4	-7.9 ± 0.3	-4.1 ± 1.8	-1.6 ± 0.5
1C6	-12.7 ± 0.1	-11.3 ± 0.9	-4.1 ± 1.6	-1.4 ± 0.8	-12.1 ± 0.1	-11.5 ± 0.4	-11.4 ± 0.2	-5.1 ± 2.7	-0.9 ± 0.7
2G3	-21.1 ± 0.1	-16.8 ± 3.5	-5.2 ± 2.3	-1.6 ± 0.6	-20.7 ± 0.1	-20.2 ± 0.1	-18.6 ± 1.0	-9.7 ± 1.4	-1.0 ± 0.8
2A4	-17.9 ± 0.1	-15.4 ± 1.8	-4.2 ± 2.9	-1.4 ± 0.6	-17.6 ± 0.0	-16.7 ± 0.2	-17.0 ± 0.2	-10.9 ± 2.0	-0.8 ± 0.4
2T5	-9.6 ± 0.1	-7.9 ± 0.5	-2.4 ± 1.5	-1.6 ± 0.6	-8.0 ± 0.4	-6.5 ± 0.1	-7.1 ± 0.2	-2.8 ± 1.4	-1.0 ± 0.3
2C6	-12.5 ± 0.0	-6.8 ± 2.9	-3.8 ± 2.5	-2.2 ± 0.6	-12.0 ± 0.5	-10.7 ± 0.3	-10.2 ± 0.7	-4.1 ± 2.4	-0.6 ± 0.3
AZP	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
1A3	-13.8 ± 0.2	-3.8 ± 0.9	-5.1 ± 1.5	-1.7 ± 0.2	-9.2 ± 0.4	-9.1 ± 0.3	-9.4 ± 0.9	-4.4 ± 1.0	-1.3 ± 0.6
1A4	-13.8 ± 0.2	-5.1 ± 1.4	-3.0 ± 1.2	-1.4 ± 0.3	-10.3 ± 0.3	-9.1 ± 0.5	-11.1 ± 0.3	-3.0 ± 0.3	-1.2 ± 0.5
1T5	-9.7 ± 0.1	-4.1 ± 1.8	-1.2 ± 0.5	-1.2 ± 0.3	-9.6 ± 0.1	-7.5 ± 0.6	-9.3 ± 0.1	-0.7 ± 0.6	-0.8 ± 0.3
1T6	-9.9 ± 0.2	-4.9 ± 1.4	-1.5 ± 0.4	-1.2 ± 0.4	-9.5 ± 0.1	-8.8 ± 0.4	-9.6 ± 0.1	-1.3 ± 0.6	-0.3 ± 0.1
2A3	-13.9 ± 0.1	-5.2 ± 2.5	-2.8 ± 1.0	-2.0 ± 0.1	-13.2 ± 0.2	-11.1 ± 0.7	-13.2 ± 0.4	-5.2 ± 1.2	-2.7 ± 0.5
2A4	-13.4 ± 0.1	-5.6 ± 2.8	-2.6 ± 0.7	-2.0 ± 0.5	-11.3 ± 0.3	-11.4 ± 0.6	-13.1 ± 0.2	-6.2 ± 1.5	-2.0 ± 0.4
2T5	-9.8 ± 0.0	-4.1 ± 2.1	-2.0 ± 0.8	-1.1 ± 0.6	-6.4 ± 0.1	-5.9 ± 0.4	-6.6 ± 0.2	-2.5 ± 0.5	-1.4 ± 0.5
2T6	-10.3 ± 0.0	-2.8 ± 1.8	-1.5 ± 0.8	-1.5 ± 0.3	-8.0 ± 0.2	-3.6 ± 0.7	-6.1 ± 0.2	-2.1 ± 0.5	-1.5 ± 0.3

Table S4: Inter strand stacking interaction energies of the central four base pairs (kcal/mol) of the DNA molecules present in the two binary complexes obtained from different MD simulations.

	DNA (alone)				DNA (complexed)				
AZP	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
1G3	-5.6 ± 0.2	-3.5 ± 0.9	-5.0 ± 1.5	-0.0 ± 0.0	-0.9 ± 0.4	-1.9 ± 0.1	-1.8 ± 0.4	-2.6 ± 0.3	0.2 ± 0.1
1A4	-1.2 ± 0.1	-1.0 ± 0.0	-0.5 ± 0.3	-0.0 ± 0.0	-0.2 ± 0.0	-0.7 ± 0.1	-0.5 ± 0.0	-1.4 ± 0.6	-1.0 ± 0.6
1T5	0.7 ± 0.0	0.3 ± 0.1	-0.1 ± 0.1	-0.0 ± 0.0	0.3 ± 0.1	-0.5 ± 0.1	-0.3 ± 0.1	-0.3 ± 0.1	-0.4 ± 0.2
1C6	2.4 ± 0.0	1.5 ± 0.8	0.1 ± 0.3	-0.1 ± 0.0	2.7 ± 0.1	2.5 ± 0.1	1.9 ± 0.2	-0.1 ± 0.4	-0.7 ± 0.3
2G3	-5.4 ± 0.1	-4.4 ± 0.9	-0.9 ± 0.9	-0.1 ± 0.1	-6.7 ± 0.2	-6.1 ± 0.7	-7.4 ± 0.6	-7.2 ± 0.4	-2.1 ± 1.2
2A4	-1.3 ± 0.0	-1.6 ± 0.4	-0.5 ± 0.3	-0.1 ± 0.0	-1.2 ± 0.1	-1.6 ± 0.1	-1.3 ± 0.2	-1.7 ± 0.5	-1.5 ± 0.6
2T5	0.6 ± 0.1	-0.7 ± 0.6	-0.2 ± 0.1	-0.0 ± 0.0	-0.1 ± 0.5	-1.3 ± 0.2	-1.0 ± 0.2	-1.7 ± 0.4	-0.2 ± 0.1
2C6	2.3 ± 0.1	1.1 ± 0.7	-0.2 ± 0.7	-0.0 ± 0.0	2.2 ± 0.0	1.9 ± 0.2	1.8 ± 0.3	-0.0 ± 0.6	-0.1 ± 0.1
AZP	**300K**	**360K**	**420K**	**480K**	**300K**	**360-1K**	**360-2K**	**420K**	**480K**
1A3	-4.3 ± 0.1	-2.2 ± 1.6	-0.1 ± 0.1	-0.0 ± 0.0	-2.3 ± 0.1	-3.8 ± 1.3	-2.1 ± 0.4	-0.0 ± 0.0	-0.3 ± 0.3
1A4	-3.2 ± 0.1	-1.5 ± 1.1	-0.0 ± 0.0	-0.1 ± 0.0	-1.7 ± 0.1	-2.8 ± 0.5	-1.3 ± 0.1	-0.0 ± 0.0	-0.2 ± 0.1
1T5	-1.2 ± 0.0	-0.6 ± 0.4	-0.2 ± 0.2	-0.5 ± 0.5	-1.3 ± 0.1	-2.7 ± 0.4	-1.6 ± 0.0	-0.0 ± 0.0	-0.1 ± 0.1
1T6	-2.8 ± 0.1	-1.0 ± 0.7	-0.2 ± 0.2	-0.1 ± 0.1	-2.2 ± 0.0	-2.0 ± 0.3	-2.2 ± 0.1	-0.0 ± 0.0	-0.1 ± 0.1
2A3	-4.4 ± 0.0	-1.3 ± 0.9	-0.2 ± 0.2	-0.5 ± 0.5	-3.8 ± 0.2	-5.2 ± 0.2	-4.3 ± 0.2	-0.1 ± 0.0	-0.1 ± 0.1
2A4	-3.3 ± 0.0	-1.0 ± 0.7	-0.0 ± 0.0	-0.1 ± 0.1	-3.5 ± 0.1	-3.3 ± 0.5	-3.1 ± 0.2	-0.0 ± 0.0	-0.0 ± 0.0
2T5	-1.3 ± 0.0	-0.5 ± 0.4	-0.1 ± 0.0	-0.0 ± 0.0	-2.2 ± 0.1	-1.4 ± 0.3	-1.2 ± 0.4	-0.0 ± 0.0	-0.3 ± 0.3
2T6	-2.7 ± 0.1	-1.2 ± 1.0	-0.0 ± 0.0	-0.2 ± 0.1	-1.4 ± 0.0	-3.2 ± 0.6	-2.6 ± 0.5	0.0 ± 0.0	-0.2 ± 0.1

Table S5: Average interaction energies (kcal/mol) of the Sac7d protein, with the base and backbone of the DNA of the nucleotides shown in Figure 5.

	AZP			AZQ		
	300	**360-1**	**360-2**	**300**	**360-1**	**360-2**
N1a-base	-6.4 ± 0.9	-7.1 ± 1.1	-7.6 ± 1.0	-7.9 ± 0.4	-6.1 ± 0.1	-5.4 ± 1.1
N1a-bkb	-113.5 ± 4.1	-104.7 ± 2.0	-106.7 ± 2.4	-109.0 ± 2.3	-111.5 ± 1.7	-109.0 ± 1.1
N2a-base	-0.5 ± 3.8	5.0 ± 0.7	4.3 ± 1.6	-13.4 ± 0.3	-11.7 ± 0.9	-7.1 ± 0.1
N2a-bkb	-142.4 ± 4.6	-124.5 ± 2.2	-123.5 ± 1.5	-124.5 ± 1.3	-137.7 ± 4.3	-119.4 ± 2.6
N3a-base	-7.2 ± 0.4	-6.9 ± 0.4	-6.7 ± 0.1	-7.8 ± 0.2	-14.5 ± 0.6	-8.0 ± 0.1
N3a-bkb	-180.2 ± 4.3	-154.6 ± 2.4	-150.9 ± 2.6	-148.8 ± 1.8	-183.7 ± 7.6	-154.3 ± 3.7
N4a-base	-10.7 ± 1.6	-10.3 ± 0.3	-9.3 ± 0.5	-11.0 ± 0.4	-8.6 ± 0.3	-9.3 ± 0.8
N4a-bkb	-201.9 ± 2.5	-193.7 ± 6.1	-185.3 ± 4.6	-150.7 ± 6.7	-194.4 ± 2.9	-203.1 ± 1.9
N5a-base	-14.8 ± 2.6	-16.9 ± 1.5	-16.4 ± 2.4	-4.1 ± 0.6	-2.4 ± 0.8	-2.7 ± 0.9
N5a-bkb	-180.3 ± 6.8	-187.4 ± 4.7	-181.3 ± 5.3	-170.8 ± 4.6	-158.7 ± 3.9	-189.7 ± 5.7
N1b-base	-6.9 ± 0.6	-5.3 ± 0.3	-6.5 ± 0.5	-9.3 ± 0.7	-4.3 ± 0.5	-7.1 ± 0.3
N1b-bkb	-183.7 ± 2.3	-170.5 ± 1.8	-179.0 ± 3.0	-166.7 ± 4.3	-186.7 ± 6.4	-225.3 ± 2.0
N2b-base	-16.3 ± 3.5	-15.1 ± 1.1	-14.0 ± 1.9	-5.0 ± 0.1	-4.9 ± 0.9	-5.1 ± 1.0
N2b-bkb	-202.7 ± 6.5	-180.4 ± 5.5	-199.5 ± 3.3	-193.5 ± 7.5	-189.9 ± 8.5	-230.3 ± 11.1
N3b-base	-10.5 ± 0.5	-12.4 ± 0.4	-11.3 ± 0.7	-10.8 ± 0.7	-5.5 ± 0.4	-12.3 ± 0.9
N3b-bkb	-185.4 ± 3.1	-167.2 ± 8.5	-193.3 ± 10.7	-183.6 ± 9.7	-184.8 ± 7.2	-181.9 ± 3.7
N4b-base	-6.8 ± 0.4	-7.7 ± 0.4	-7.5 ± 0.4	-8.2 ± 0.3	-6.0 ± 0.3	-6.4 ± 0.3
N4b-bkb	-140.5 ± 2.7	-128.8 ± 4.1	-140.4 ± 7.2	-124.7 ± 2.3	-134.5 ± 4.0	-126.6 ± 3.2
N5b-base	10.1 ± 1.2	11.1 ± 0.7	10.7 ± 0.7	-3.4 ± 0.1	-3.2 ± 0.6	-3.7 ± 0.2
N5b-bkb	-102.4 ± 1.1	-96.7 ± 1.6	-100.3 ± 2.4	-91.3 ± 0.8	-102.3 ± 2.0	-98.6 ± 1.3

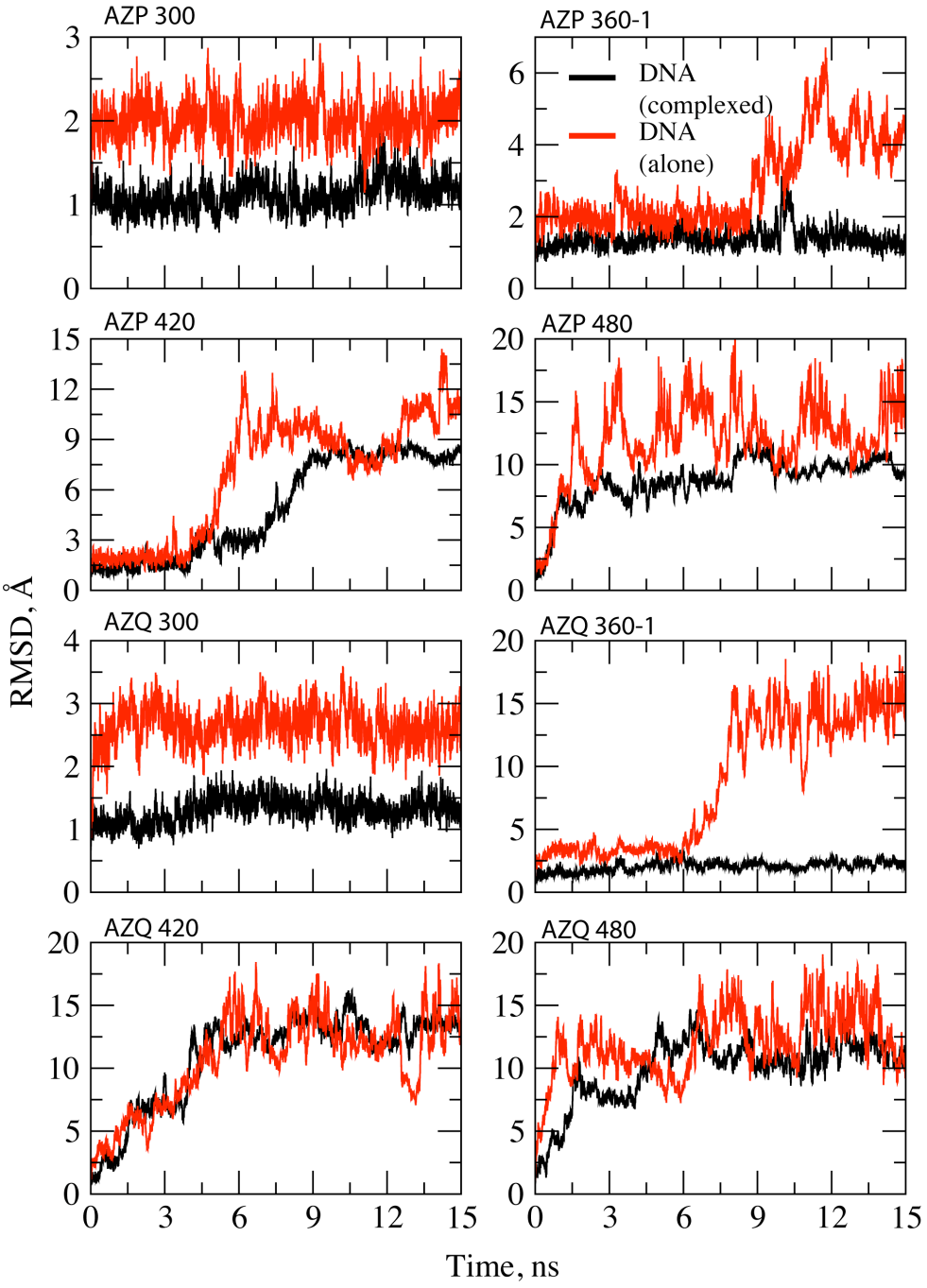

Figure S1: The time series of the RMSD values obtained for the DNA molecules in the MD simulations of DNA alone and protein-DNA complexes at different temperatures.

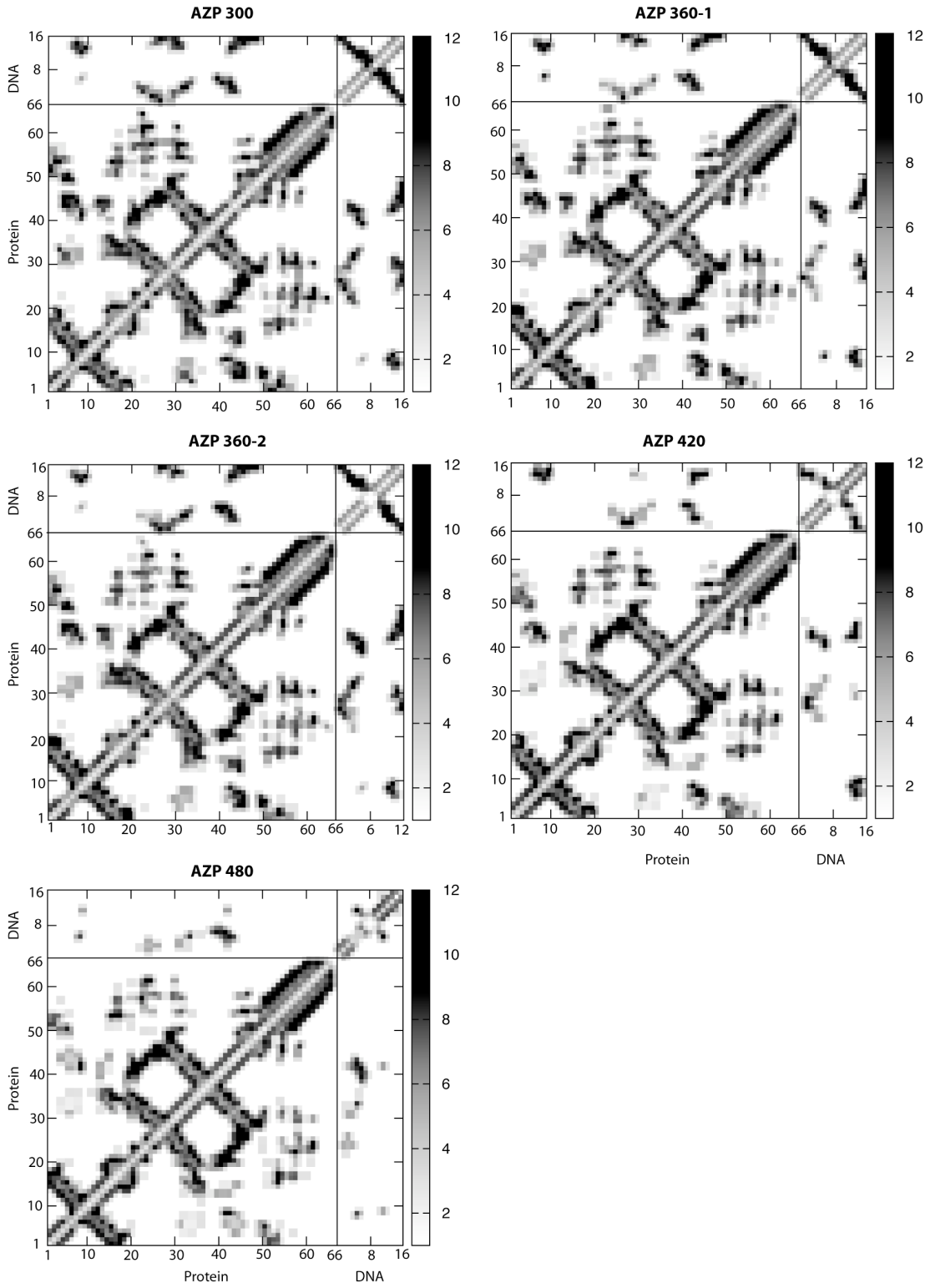

Figure S2: Contact maps showing the inter residue/nucleotide distances that are less than 12 Å calculated using the last 3 ns of the MD simulations on the AZP binary complex at different temperatures.

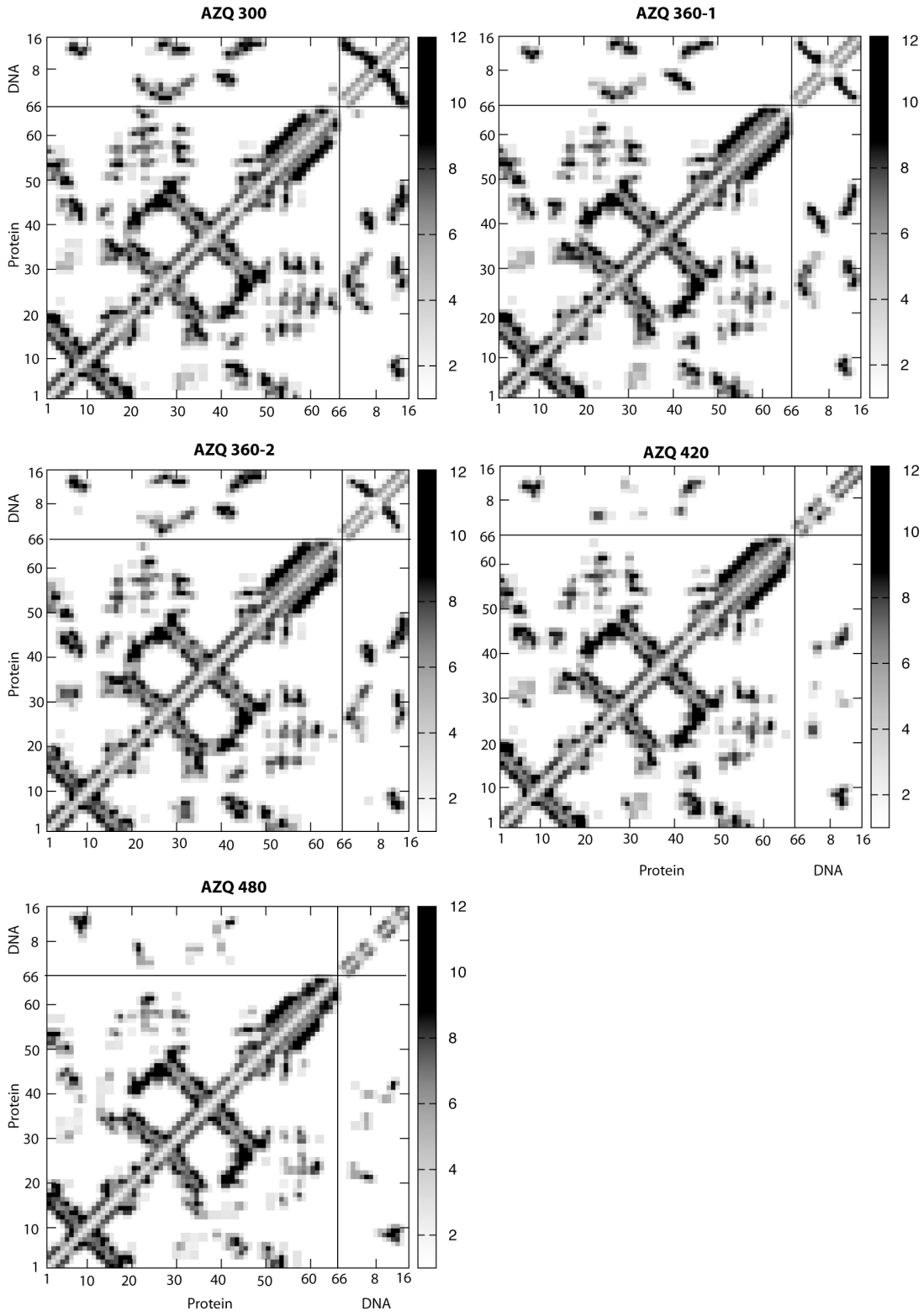

Figure S3: Contact maps showing the inter residue/nucleotide distances that are less than 12 Å calculated using the last 3 ns of the MD simulations on the AZQ binary complex at different temperatures.

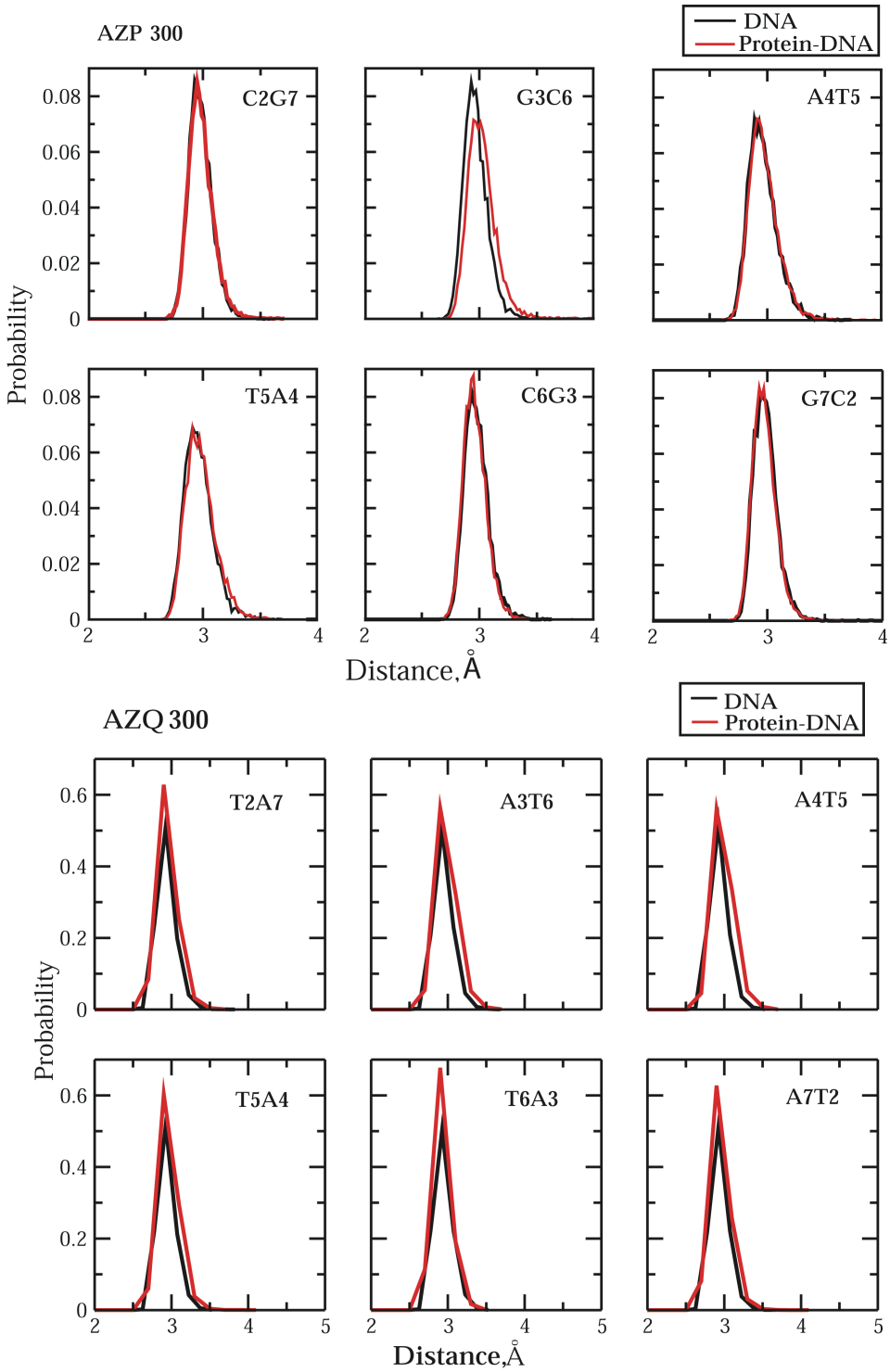

Figure S4: Probability distributions corresponding to the N1(gua/ade)-N3(cyt/thy) distances of the central six base pairs of the DNA in the DNA alone (black), and binary (red) systems at 300 K.

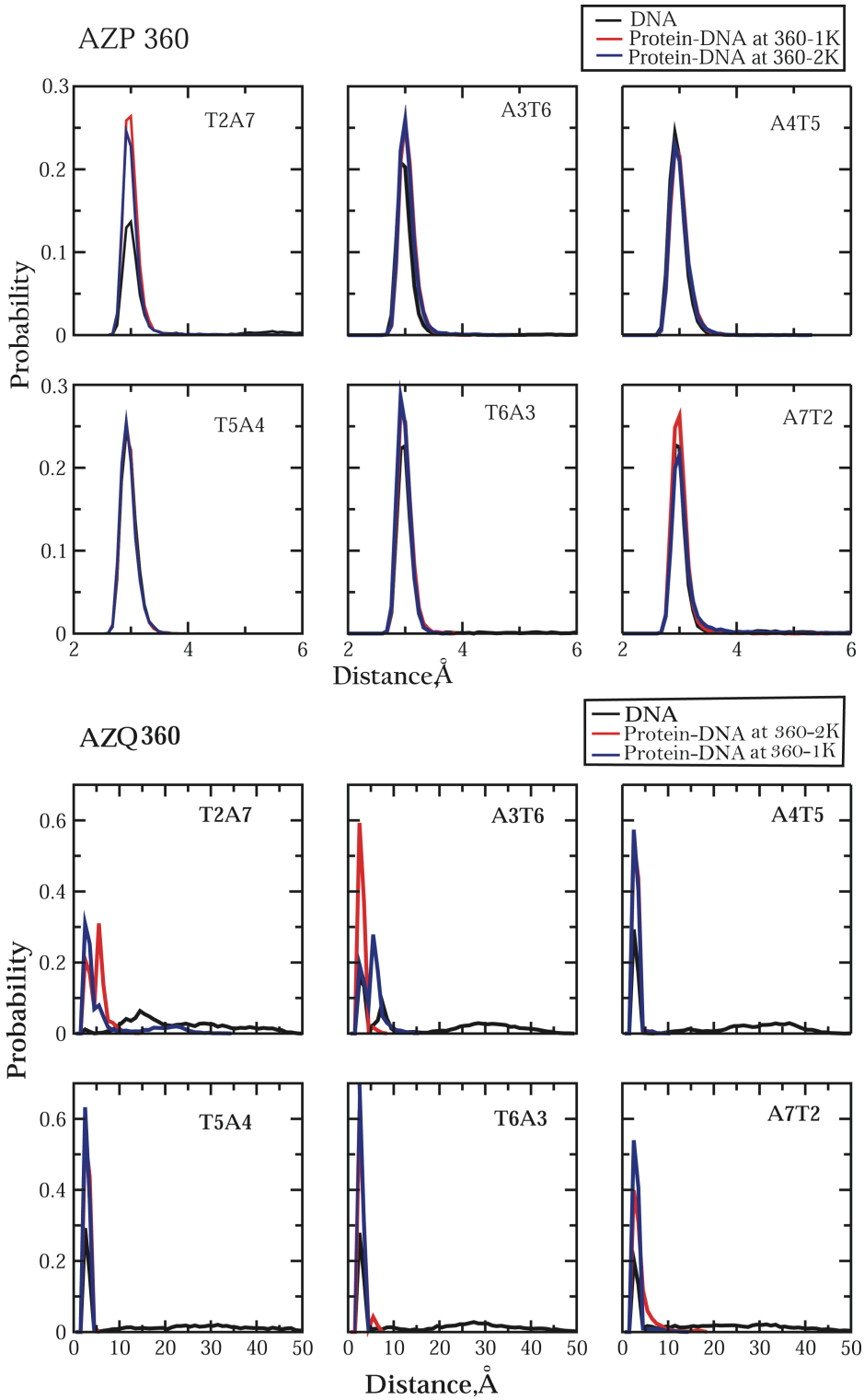

Figure S5: Probability distributions corresponding to the N1(gua/ade)-N3(cyt/thy) distances of the central six base pairs of the DNA in the DNA alone (black), and binary (red, and blue) systems at 360 K.

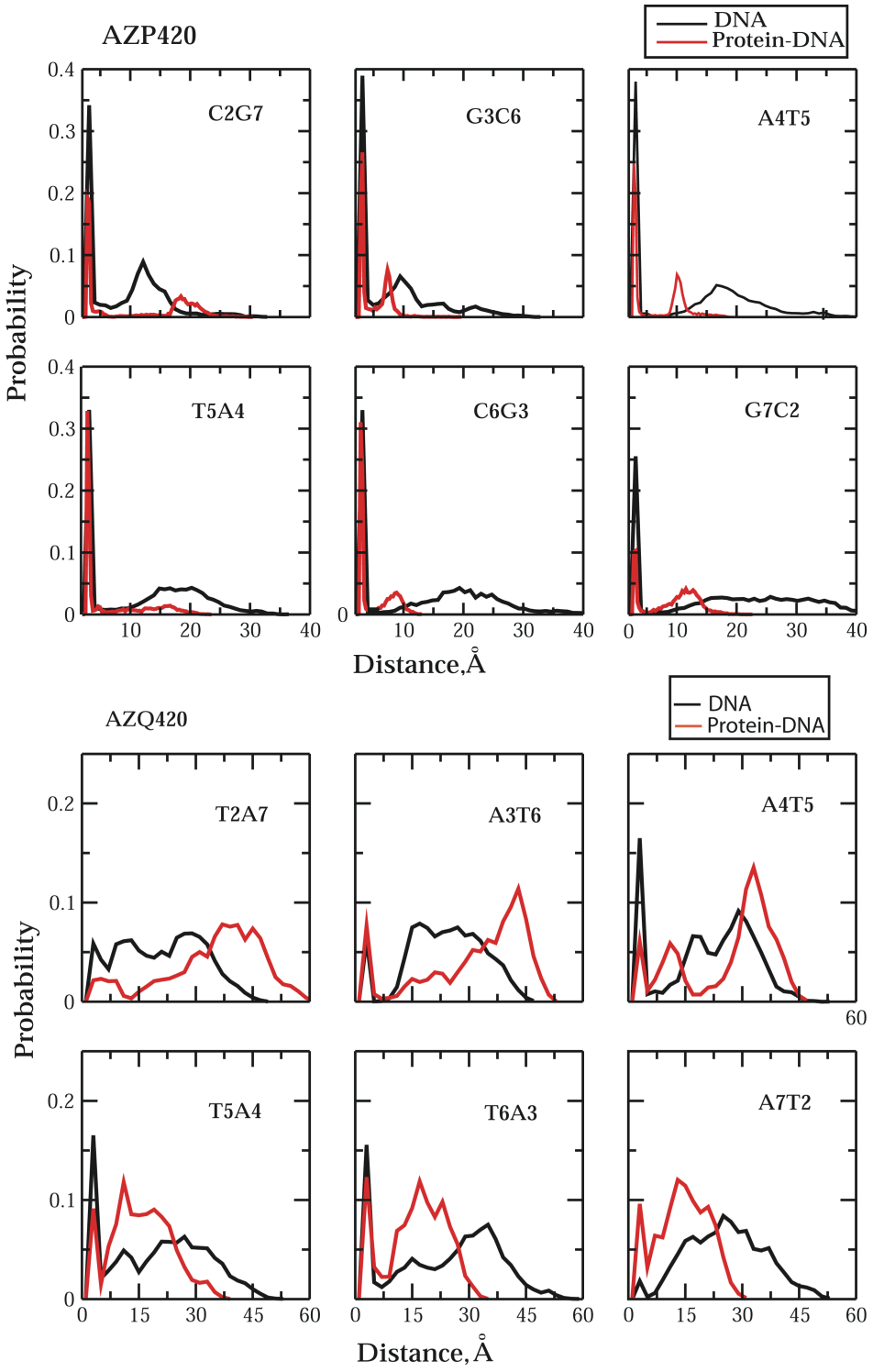

Figure S6: Probability distributions corresponding to the N1(gua/ade)-N3(cyt/thy) distances of the central six base pairs of the DNA in the DNA alone (black), and binary (red) systems at 420 K.

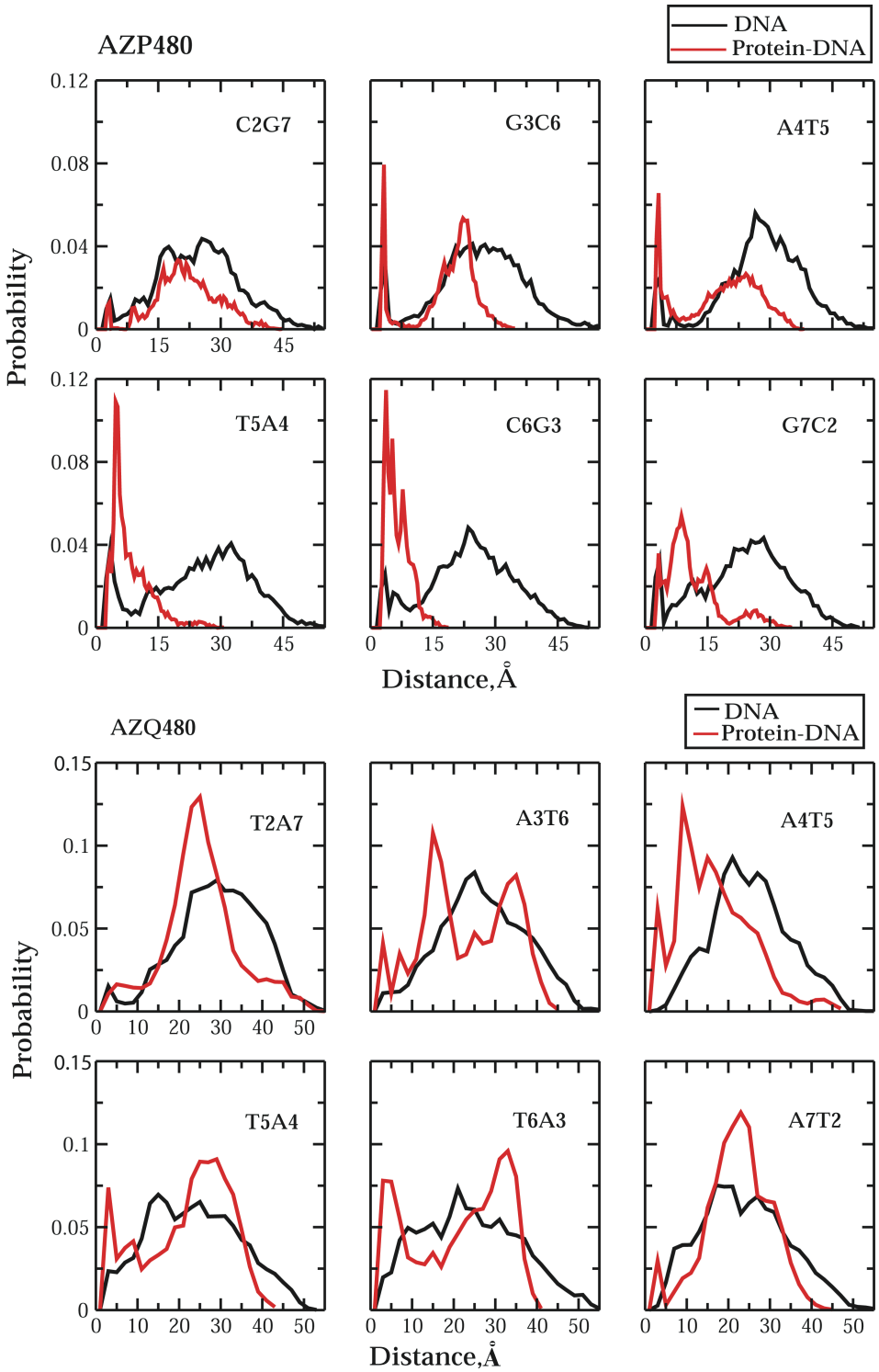

Figure S7: Probability distributions corresponding to the N1(gua/ade)-N3(cyt/thy) distances of the central six base pairs of the DNA in the DNA alone (black), and binary (red) systems at 300 K.