



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 73 (2017)

Supporting information for article:

Crystal structure of the DNA sequence d(CGTGAATTCACG)₂ with DAPI

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Table S1 *X3DNA* (Zheng *et al.*, 2009) results for base-pair morphology: shear, stretch, stagger, buckle, opening and propeller twist values in 5t4w and 5ju4 DNA crystal structures.

	Pair	Shear		Stretch		Stagger		Buckle		Propeller		Opening	
		5T4W	5JU4	5T4W	5JU4	5T4W	5JU4	5T4W	5JU4	5T4W	5JU4	5T4W	5JU4
1-24	C-G	0.05	0.39	-0.05	-0.22	0.07	-0.13	-0.20	4.99	-11.90	-10.24	-2.10	0.45
2-23	G-C	-0.04	-0.32	-0.23	-0.31	0.22	-0.04	-0.21	-4.24	-18.61	-3.12	-3.28	-6.15
3-22	T-A	0.20	-0.3	-0.32	-0.07	0.05	-0.27	-3.82	4.58	-5.78	-6.3	0.62	-2.78
4-21	G-C	-0.45	-0.48	-0.34	-0.18	0.04	-0.07	11.92	10.06	-5.93	-5.61	3.04	0.62
5-20	A-T	-0.38	0.13	-0.15	-0.05	-0.04	-0.12	6.05	8.06	-14.74	-11.91	5.33	2.01
6-19	A-T	0.28	-0.08	-0.11	-0.12	-0.00	0.09	4.60	3	-21.83	-17.08	3.85	3.61
7-18	T-A	0.12	-0.02	0.01	-0.03	0.21	0.08	-2.69	-0.63	-22.16	-15.28	9.28	1.8
8-17	T-A	0.43	0.02	-0.34	-0.11	0.04	0.09	-4.53	-3.97	-14.96	-15.32	5.61	3.81
9-16	C-G	0.18	0.26	-0.16	-0.06	0.14	0.09	-14.58	-15.17	-7.94	-12.21	1.83	-0.49
10-15	A-T	-0.29	-0.08	-0.25	-0.22	0.08	0.16	5.32	-0.06	-6.41	-6.92	-1.43	3.8
11-14	C-G	-0.17	0.04	0.05	-0.08	0.31	0.15	5.47	1.79	-21.55	-16.8	-8.78	0.09
12-13	G-C	0.12	-0.19	-0.12	-0.16	0.23	-0.06	6.15	10.34	-6.21	16.47	-6.65	-4.39