



STRUCTURAL
BIOLOGY

Volume 72 (2016)

Supporting information for article:

DNA polymorphism in crystals: three stable conformations for the decadeoxynucleotide d(GCATGCATGC)

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Table S1 Helical parameters of B-type helix

Base pair	X-dip	Y-dip	H-rise	Incl.	Tip	H-Twist
G1-C10	0	0	0	0	0	0
C2-G9	1.99	-0.34	3.21	-4.51	-0.27	39.21
A3-T8	4.33	0.25	2.88	-9.23	2.78	46.96
T4-A7	0.57	-0.77	3.60	10.00	7.15	30.29
G5-C6	3.62	0.52	3.04	-7.75	-2.65	46.09
C6-G5	1.19	0.19	3.08	9.96	-0.45	34.01
A7-T4	3.61	-0.26	3.19	-4.63	1.45	49.06
T8-A3	-0.93	0.26	3.42	19.21	-3.42	24.66
G9-C2	4.38	-0.06	2.74	-9.18	-3.76	48.24
C10-G1	1.51	0.24	3.34	-4.36	1.29	41.83
Average	2.25	0.00	3.17	-0.06	0.23	40.04
(average of fiber B-DNA)	(0.11)	(0.00)	(3.38)	(-4.52)	(0.00)	(36.23)

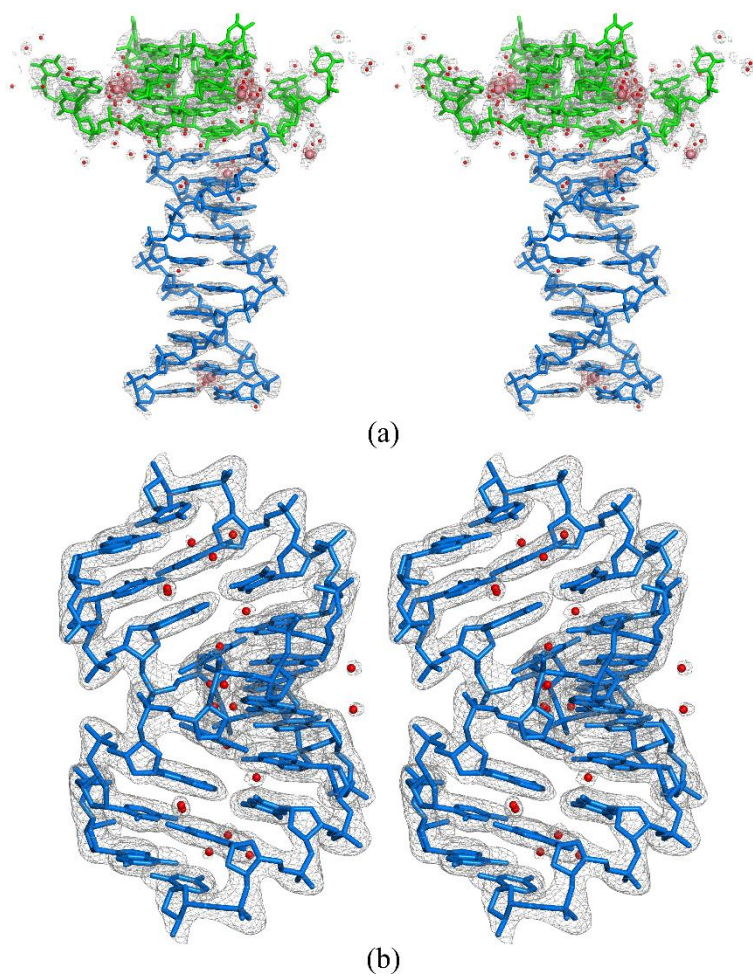


Figure S1 (a) The asymmetric unit of the tetragonal crystal along with the $(2F_o - F_c)$ electron density map (grey) and the anomalous difference map (red). Maps contoured at 1σ and 5σ level, respectively. (b) The A-type duplex in the hexagonal crystal along with $(2F_o - F_c)$ electron density map contoured at 1σ level. Both the reference molecule and its symmetry mate are shown.

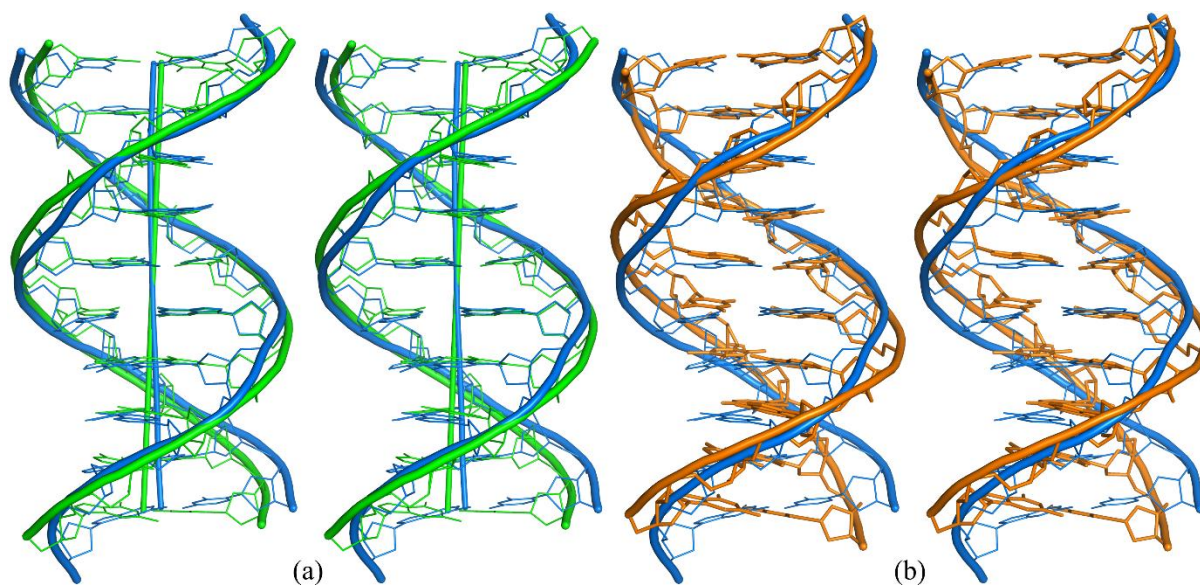


Figure S2 (a) Wall-eyed stereo representations of the least-square superposition of the B-type helix in the tetragonal crystal (blue), with fiber B-DNA (green). (b) B-type helix (blue) with the Drew-Dickerson dodecamer (orange, PDB entry; 1bna (Drew *et al.*, 1981)).

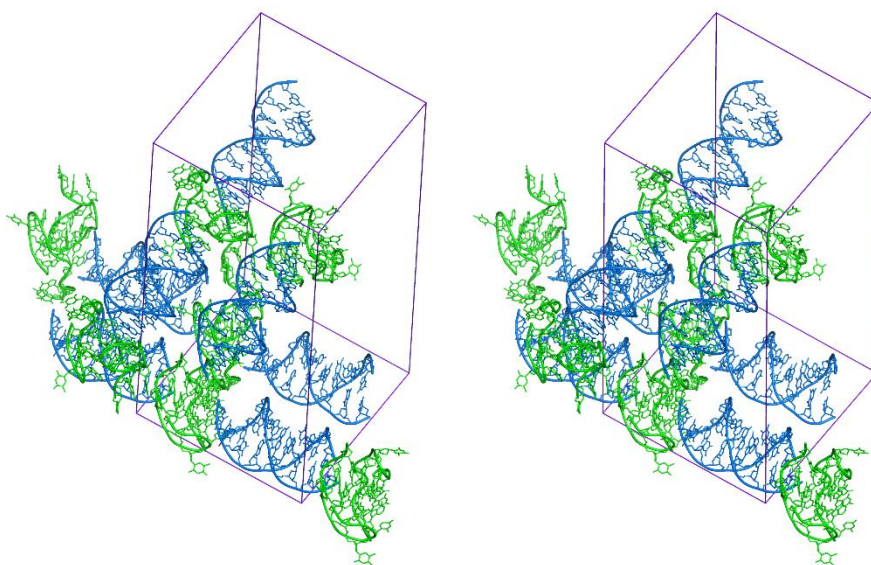


Figure S3 Wall-eyed stereo-view of the crystal packing in the tetragonal crystal system.

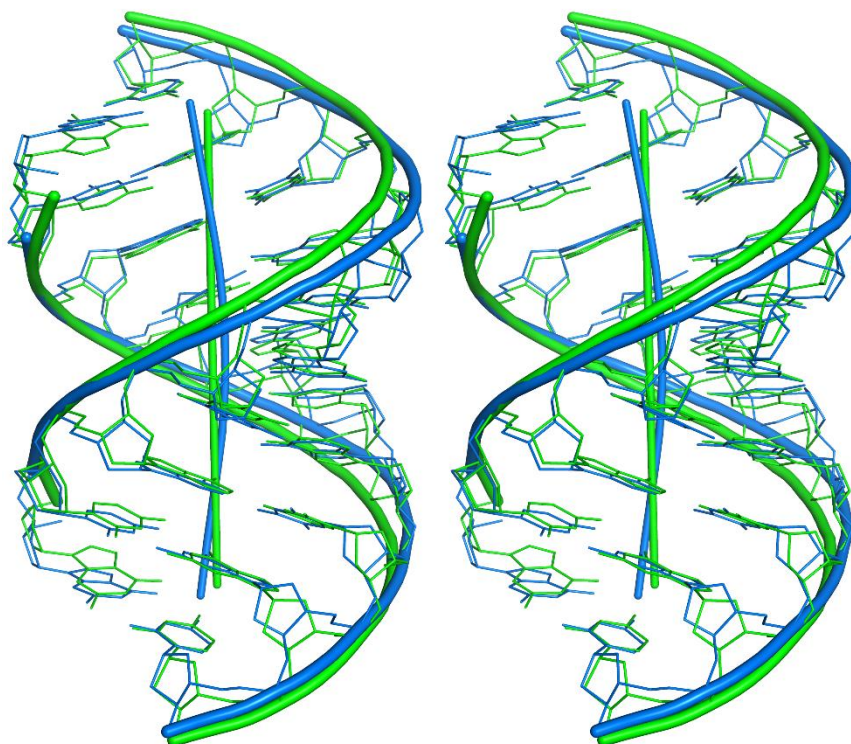


Figure S4 Least-squares superposition of the A-type helix (blue) with the fiber A-DNA (green). The helical axes are indicated.

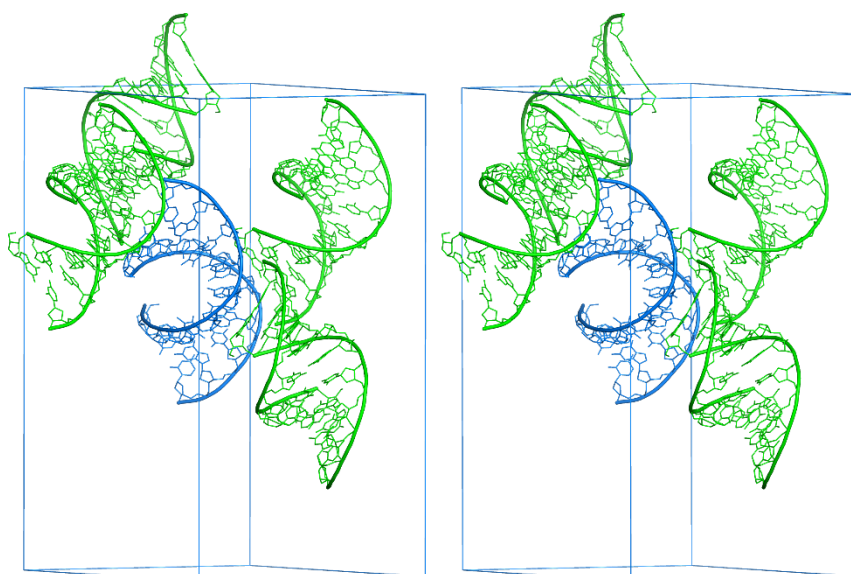


Figure S5 Wall-eyed stereo-view of the crystal packing in the hexagonal crystal system.

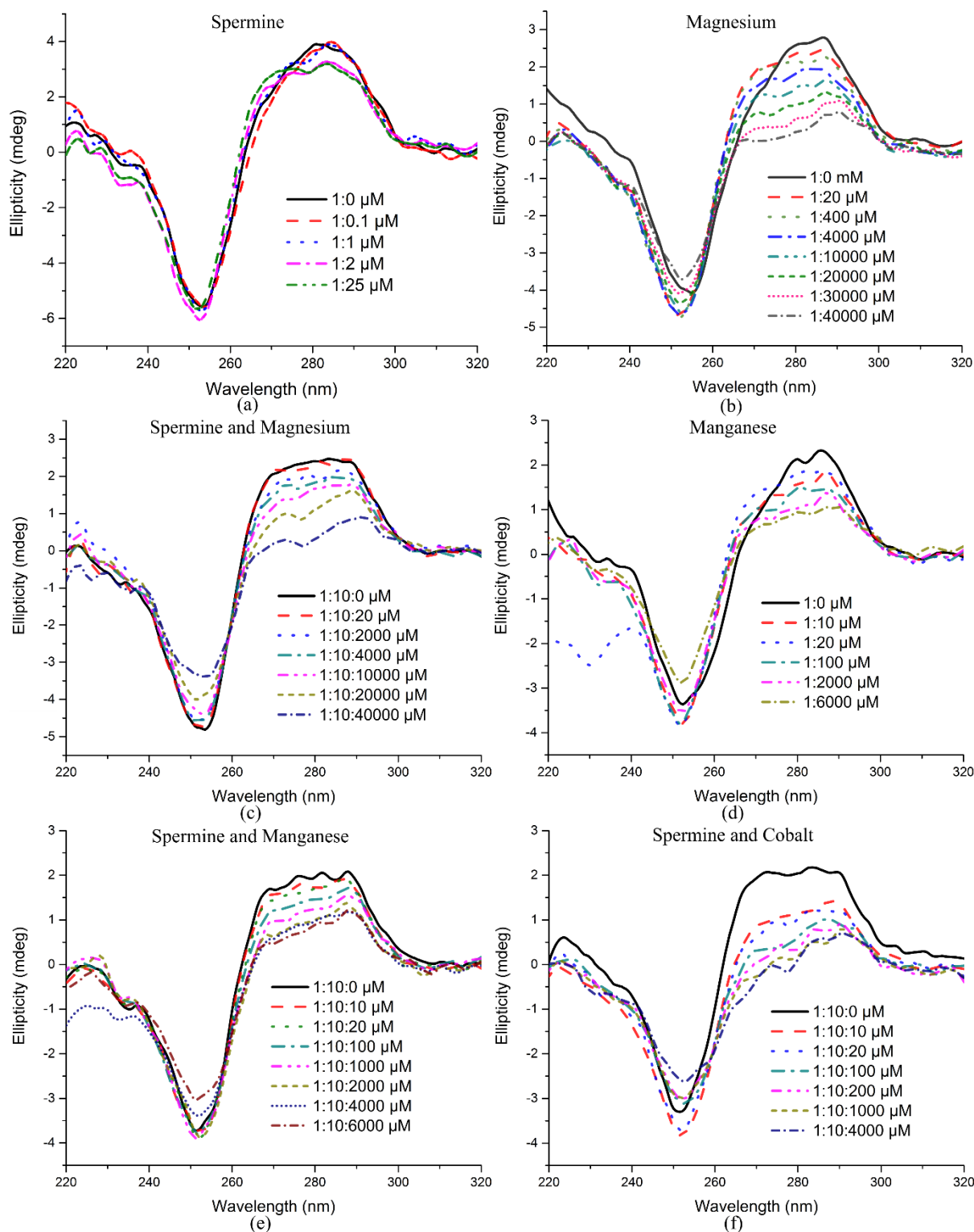


Figure S6 CD spectra of the DNA decamer titrated against spermine and various metal ions. (a) Spermine. (b) Magnesium. (c) Spermine and Magnesium. (d) Manganese. (e) Spermine and Manganese. (f) Spermine and Cobalt.