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Supporting information for article:

Crystal structure of d(CCGGGGTACCCGG)₂ at 1.4 Å resolution

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Table S1 Overall $R_{\text{work}}/R_{\text{free}}$ of paired refinement

High resolution limit for R value calculation (Å)	High resolution limit for refinement (Å)			
	1.7	1.6	1.5	1.4
1.7	0.2019/0.2150	0.2065/0.2108	0.2101/0.2274	0.2156/0.2121
1.6		0.2158/0.2404	0.220/0.2387	0.2262/0.2264
1.5			0.2240/0.2673	0.2304/0.2249
1.4				0.2219/0.2443

Base-pair step parameters.

Base-pair step	Rise (Å)	Twist (°)	Tilt (°)	Roll (°)	Incl. (°)
CC/GG	3.23	26.04	-2.01	-3.02	-6.65
CG/CG	3.48	26.36	0.65	-3.25	-7.10
GG/CC	3.53	32.96	-0.57	1.23	2.17
GG/CC	3.32	27.89	-2.25	10.23	20.34
GG/CC	3.38	31.94	2.04	12.98	22.44
GT/AC	3.10	31.90	-1.09	10.80	18.98
TA/TA	2.99	32.51	-0.97	3.80	6.76
AC/GT	3.28	28.68	0.21	4.38	8.77
CC/GG	3.76	38.20	-7.68	10.97	16.17
CC/GG	3.14	25.85	3.96	4.59	10.08
CC/GG	3.31	30.52	1.01	0.75	1.42
CG/CG	3.56	27.38	-1.65	-1.17	-2.47
GG/CC	3.37	26.66	1.90	-0.19	-0.42

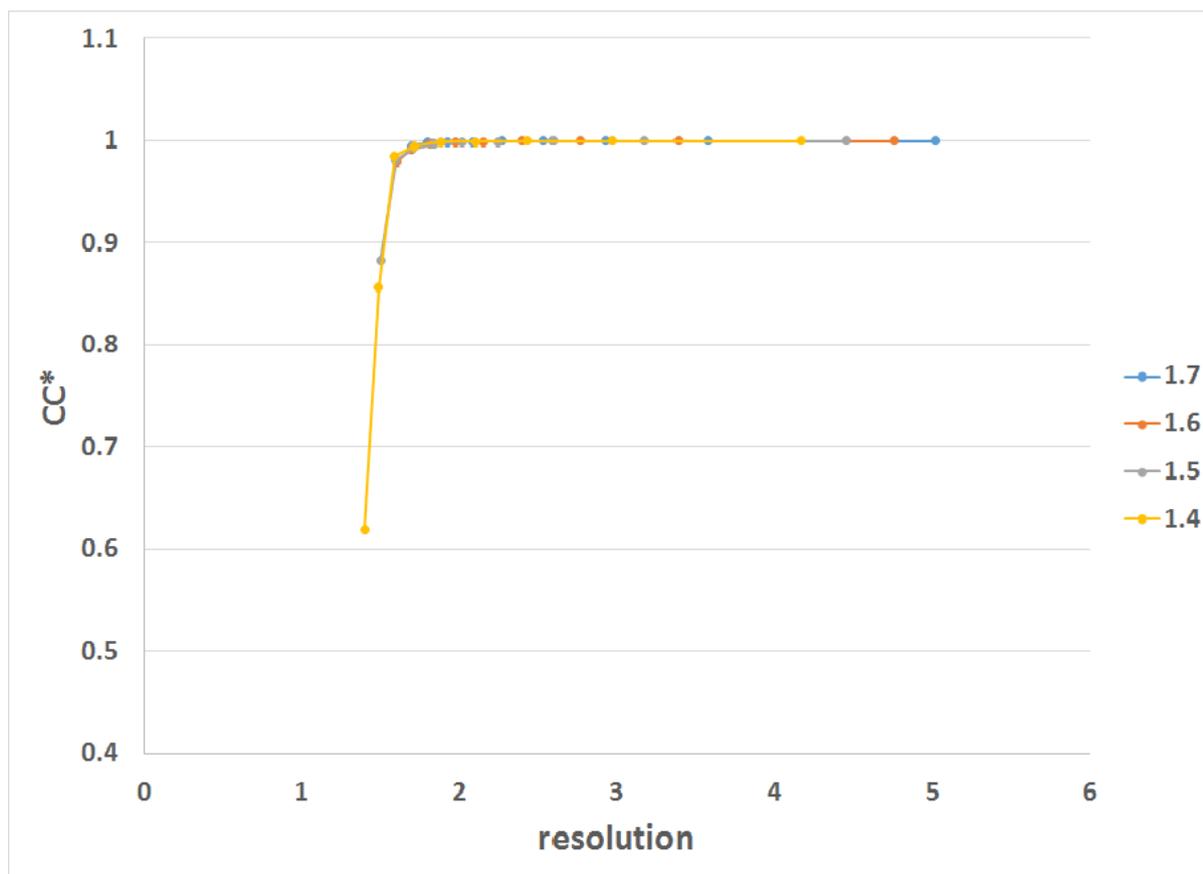


Figure S1 CC* versus resolution. $CC^* = \sqrt{2CC(1/2)} / \sqrt{1+CC(1/2)}$ (Karplus & Diederichs, 2012).

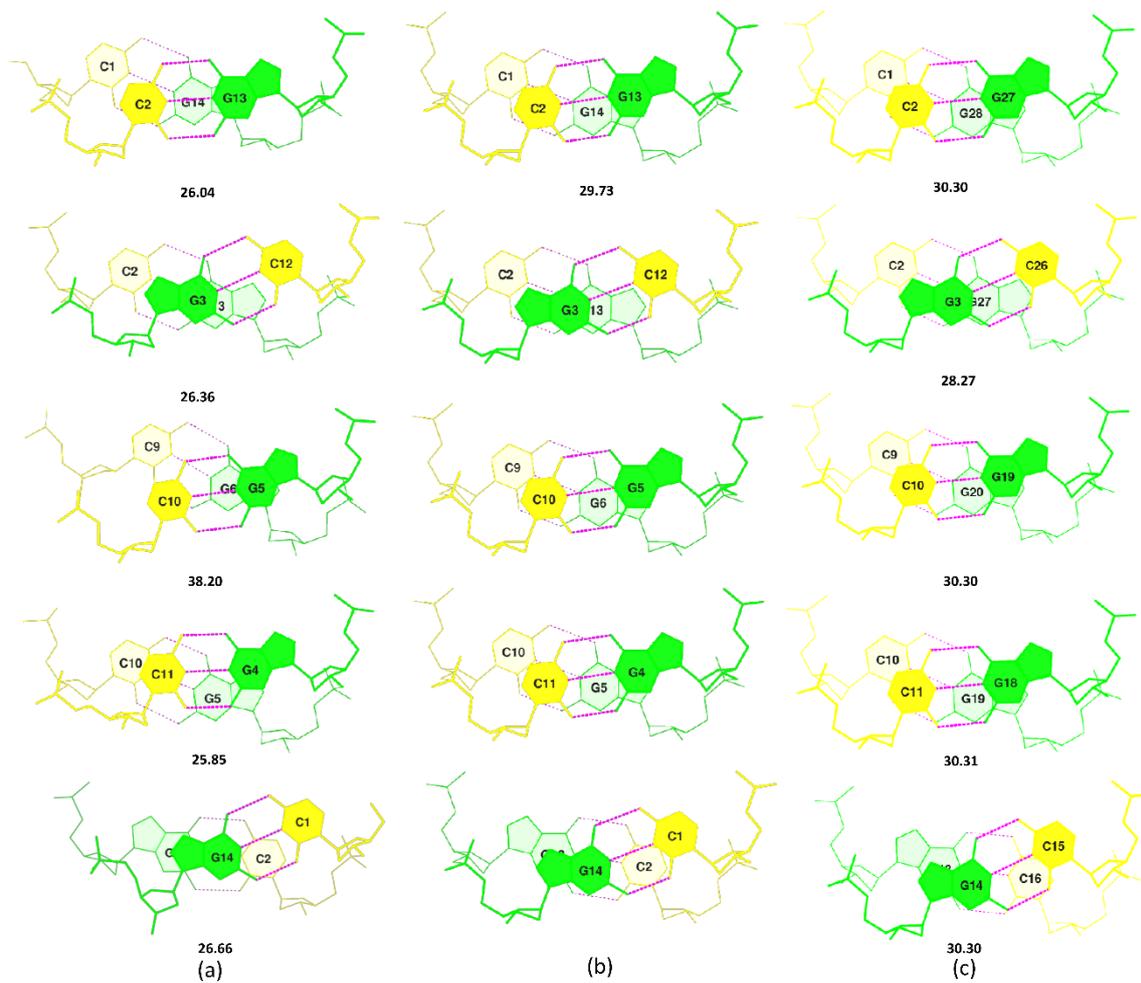


Figure S2 *w3DNA* generated images of 1st, 2nd, 9th, 10th, and 13th base-pair steps of the (a) structure (b) customized model (c) fibre A-DNA model.