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Supporting information for article:

Sequence-dependent structural changes in a self-assembling DNA oligonucleotide

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Table S1. Local base pair & base pair step parameters for A3-14 structure.

Base pair	Shear	Stretch	Stagger	Buckle	Prop-Tw	Opening	Shift	Slide	Rise	Tilt	Roll	Twist
G1-G11	5.87	-0.39	-0.09	31.53	0.08	-107.78	-	-	-	-	-	-
G2+A14*	3.19	-3.82	-0.83	43.86	-10.55	-67.89	4.31	-1.54	3.55	8.74	1.93	35.24
A3-G10	-6.79	-4.4	0.57	-23.04	-4.36	3.99	1.12	-0.08	4.21	8.44	-3.33	-23
A4-T9	0.08	-0.07	-0.11	1.84	2.38	1.15	-0.61	1.86	2.98	0.89	3.91	60.33
A5-T8	0.21	-0.02	0.21	11.24	-8.59	-0.31	-0.61	0.32	3.2	-3.55	3.06	32.43
G6-C7	-0.25	0.06	0.18	6.69	-9.95	0.97	-0.27	-0.27	3.41	-1.92	2.47	34.4
C7-G6	0.25	0.06	0.18	-6.69	-9.95	0.97	0	-0.5	3.55	0	1.5	39.57
T8-A5	-0.21	-0.02	0.21	-11.24	-8.59	-0.31	0.27	-0.27	3.41	1.92	2.47	34.4
T9-A4	-0.08	-0.07	-0.11	-1.84	2.38	1.15	0.61	0.32	3.2	3.55	3.06	32.43
G10-A3	6.79	-4.4	0.57	23.04	-4.36	3.99	0.61	1.86	2.98	-0.89	3.91	60.33
A14*+G2	-3.19	3.82	0.83	-43.86	10.55	67.89	-0.21	4.34	-0.34	167.5	-34.07	43.07
G11-G1	-5.87	-0.39	-0.09	-31.53	0.08	-107.78	-4.77	-2.21	-2.44	163.03	-51.78	24.92
A12+G1*	-2.66	6.03	-0.54	-18.69	24.92	-118.03	1.45	-0.78	3.29	5.17	-2.19	49.25
G13+G2*	3.83	-0.62	-0.54	21.33	9.96	-121.89	0.94	1.16	2.81	-0.94	7.56	49.5

* Indicates nucleotide from an adjacent duplex.

The color of the base pairs correspond to Figure 2.

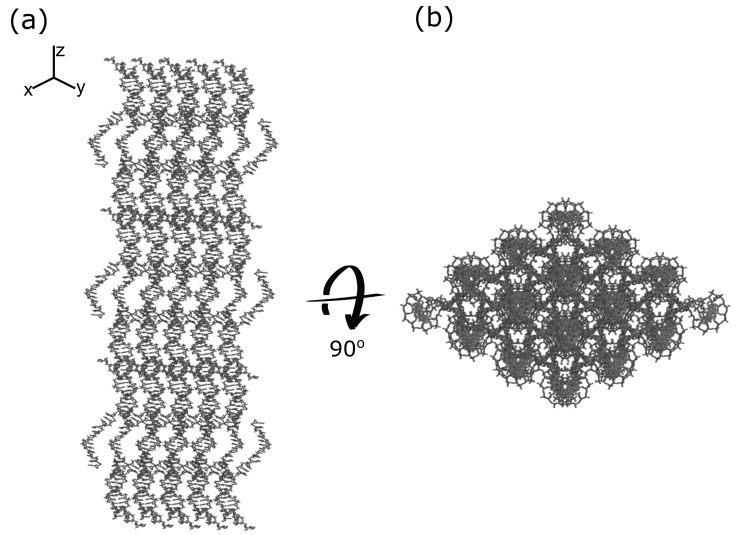

Figure S1. Crystal packing. (a) The overall 3D arrangement of the 14-mer in the crystal lattice looking perpendicular to the three-fold symmetry axis, and (b) looking down the three-fold symmetry axis, . Duplex regions are coaxially stacked with adjacent duplexes interacting only through tertiary contacts via the added A14 nucleotide.

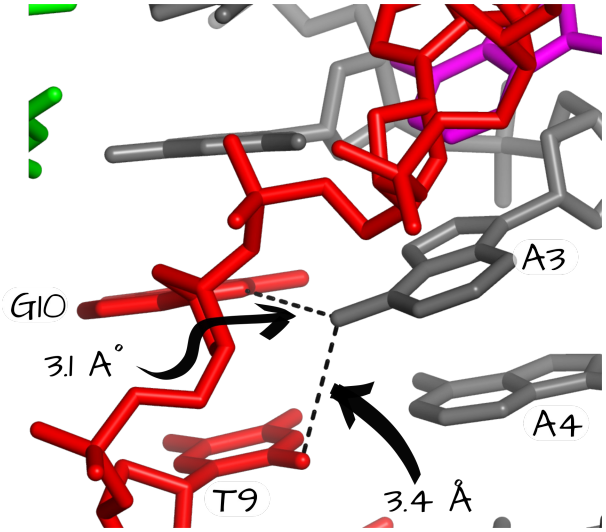

Figure S2. Potential hydrogen bond between A3 and T9. The sheared A3-G10 base pair leads to the formation of an interstrand hydrogen bond between N6 of A3 and O2 of T9, shown in dotted lines.