

SUPPLEMENTARY MATERIAL

Figure S1. The crystal packing of the complex viewed down the *c* axis. The two series of continuous pseudo-helices crossing each other delimit infinite channels parallel to the *c* axis and form successive sheets of stacked duplexes aligned along the diagonals of the *a*-*b* plane.

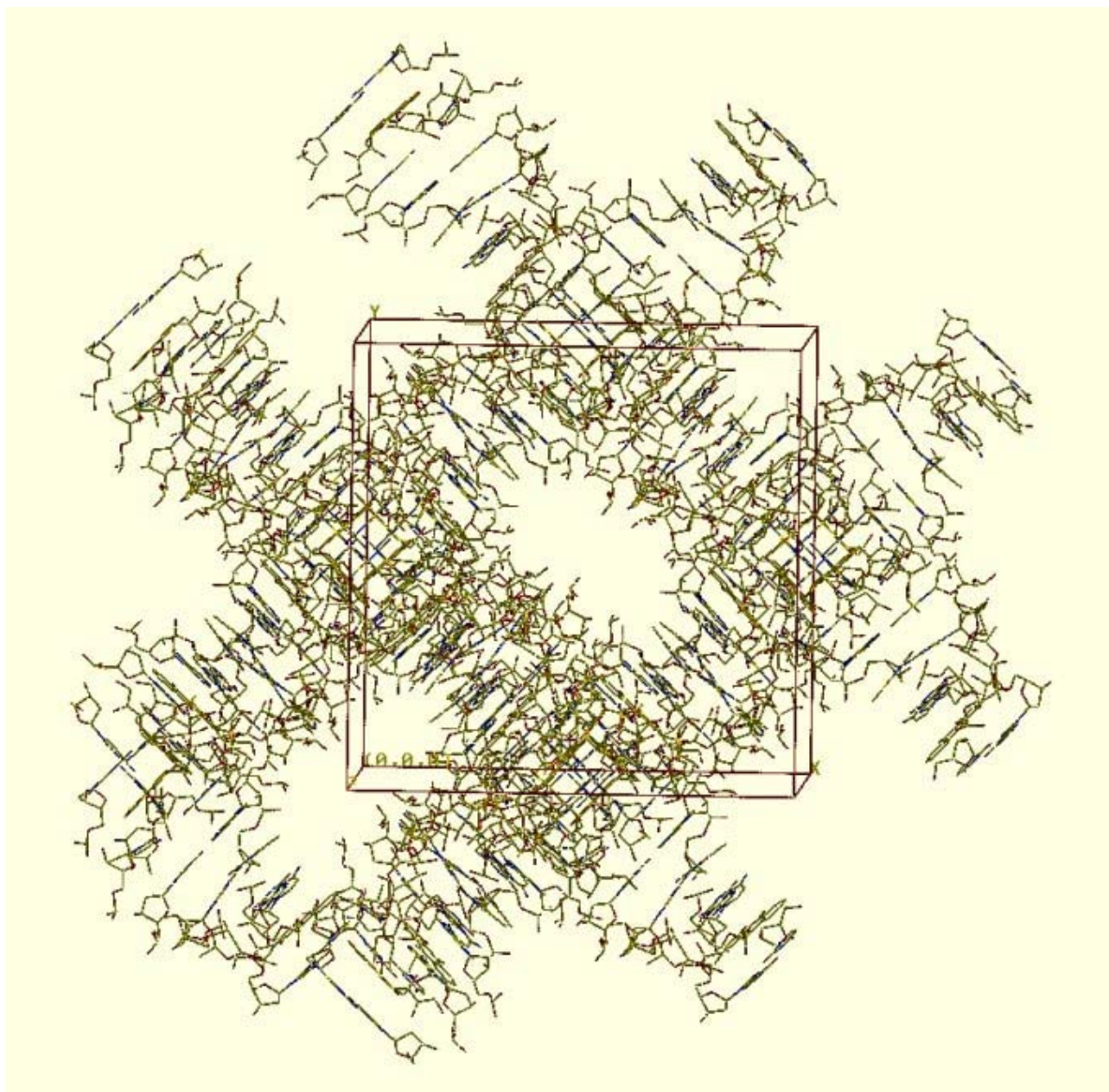


Table S1. Torsion angles and geometrical DNA helical parameters.

Selected torsion angles									
Residue	α	β	γ	δ	ϵ	ξ	χ	P	Ribose pucker
C1			155.5	150.0	-142.0	-32.4	162.2	221.0	C4'-endo
G2	-94.1	156.7	55.9	138.8	-132.6	174.0	-109.1	141.4	C1'-exo
A3	-51.4	136.1	50.9	133.0	-180.0	-99.0	-115.8	144.2	C2'-endo
T4	-53.8	166.3	46.6	117.8	-162.3	-93.8	-116.1	121.1	C1'-exo
C5	-55.9	169.8	40.2	149.3	-122.7	156.9	-75.5	153.9	C2'-endo
G6	-29.6	159.9	24.5	153.4			-78.4	174.8	C2'-endo
C7			70.5	97.0	-157.9	-75.1	-151.7	103.1	O1'-endo
G8	-77.1	-171.0	70.5	130.3	-138.8	-176.9	-99.9	144.8	C2'-endo
T9	-42.9	140.3	34.3	139.8	-177.3	-91.8	-113.4	187.4	C3'-exo
A10	-49.4	169.3	30.2	122.5	-158.7	-94.7	-106.6	134.3	C1'-exo
C11	-54.4	151.3	35.7	130.0	-86.1	159.7	-82.5	140.0	C1'-exo
G12	-92.2	170.5	60.4	143.2			-93.6	170.4	C2'-endo

Helical parameters							
Base-pair	Roll (°)	Tilt (°)	Inclin (°)	Prop Tw (°)	Buckle (°)	Helic Tw (°)	Rise (°)
C1/G12			2.3	-1.3	12.9		
	-2.7	-2.8				32.2	7.5
G2/C11			0.03	-0.8	-28.5		
	0.6	-6.8				36.2	2.7
A3/T10			-1.9	-17.8	-8.5		
	2.9	-6.0				27.8	3.3
T4/A9			-4.7	-3.0	0.98		
	6.0	7.2				33.7	3.1
C5/G8			-1.6	6.1	13.6		
	-2.8	-2.0				27.9	6.9
G6/C7			-1.5	0.3	-1.8		

These parameters were obtained from the program Curves 5.3 provided by R. Lavery (1) and are defined in accordance with EMBO workshop guidelines (2).

REFERENCES

1. Lavery, R. and Sklenar, H. (1989) Defining the structure of irregular nucleic acids: convention and principles. *J. Biomol. Struct. Dyn.*, **6**, 655–667.
2. Dickerson, R.E., Bansal, M., Calladine, C.R., Diekmann, S., Unter, W.N., Kennard, O., van Kitzing, E., Laury, R., Nelson, H.C.M., Olson, W.K., Saenger, W., Shakked, Z., Sklenar, H., Soumpasis, D.M., Tung, C.S., Wang, A.K.J. and Zurkin, W.B. (1989) Definition and nomenclature of nucleic acid structure components. *Nucleic Acids Res.*, **17**, 1797–1803.