Supplementary Table 1

Root mean squares deviation (in Å) of OrthHT1, HexHT1 and DinuHT1 with the fibre model Z-DNA (CGCGCG) and among each other upon least squares superposition of the positions of the common atoms. The rmsd of HT5, HT3 and HAT61 (d(TGCGCA)$_2$) among each other and with the structures under study are also given.

CGCGCG	0.0						
HT5	0.4	0.0					
HT3	1.3	1.3	0.0				
OrthHT1	1.1	1.1	1.4	0.0			
HexHT1	0.6	0.6	1.1	1.0	0.0		
DinuHT1	0.7	0.6	1.1	1.0	0.4	0.0	
HAT61	0.9	0.9	1.2	1.2	1.0	1.0	0.0
	CGCGCG	**HT5**	**HT3**	**OrthHT1**	**HexHT1**	**DinuHT1**	**HAT61**

Supplementary Table 2:

Base step parameters of various helices under comparison.

Sequence	**Base step**	**Tilt (°)**	**Roll (°)**	**Slide (Å)**	**Twist (°)**	**Rise (Å)**
CGCGCG	C1.G12 G2:C11	0.9	5.1	5.2	-7.4	3.8
HT5	C1.G12 G2.C11	-0.4	3.9	5.5	-14.0	4.6
HT3	C1.G12 G2.C11	5.9	-1.3	3.9	-3.4	2.6
OrthHT1	T1.A12 G2.C11	5.1	-1.4	3.3	-12.8	3.9
HexHT1	T1.A12 G2.C11	-4.6	-0.9	3.8	-14.6	3.9
CGCGCG	G2.C11 C3.G10	0.0	3.5	-0.8	-50.4	3.8
HT5	G2.C11 C3.G10	0.7	0.7	-0.8	-48.3	3.2
HT3	G2.C11 T3.A10	-5.9	-10.7	0.2	-45.2	4.2
OrthHT1	G2.C11 C3.G10	-0.2	1.9	-0.9	-49.7	3.6
HexHT1	G2.C11 C3.G10	-1.1	10.7	-0.7	-47.9	3.6
CGCGCG	C3.G10 G4.C9	-0.7	4.1	5.4	-7.7	3.7
HT5	C3.G10 G4.C9	-1.2	4.4	5.4	-10.2	3.8
HT3	T3.A10 G4.C9	-0.5	0.7	4.7	-24.5	2.5
OrthHT1	C3.G10 G4.C9	0.1	4.1	5.3	-8.1	3.7
HexHT1	C3.G10 G4.C9	0.0	-0.1	5.3	-11.0	3.6

Sequence	Base step	Tilt (°)	Roll (°)	Slide (Å)	Twist (°)	Rise (Å)
CGCGCG	G4.C9 C5.G8	0.5	1.7	-0.7	-51.8	3.6
HT5	G4:C9 T5:A8	-0.3	2.8	0.9	-48.7	3.9
HT3	G4:C9 C5:G8	-3.3	6.4	-1.4	-40.6	4.5
OrthHT1	G4:C9 C5:G8	0.0	2.5	-0.7	-50.3	3.7
HexHT1	G4:C9 C5:G8	-0.8	6.4	-0.8	-48.7	3.6
CGCGCG	C5.G8 G6.C7	-0.7	2.3	5.4	-10.7	3.8
HT5	T5:A8 G6:C7	2.6	2.3	3.4	-8.1	3.1
HT3	C5:G8 G6:C7	1.4	-6.9	5.5	-16.8	2.9
OrthHT1	C5:G8 G6:C7	-2.0	0.3	5.2	-13.2	3.7
HexHT1	C5:G8 G6:C7	-1.9	0.9	5.3	-11.5	3.8
DinuHT1	T13:G16 G14:T15	1.4	2.3	5.2	-11.5	3.7
CGCGCG	Virtual step	-0.1	-6.0	-0.9	-52.1	3.4
HT5	Virtual step	0.7	-6.3	-1.0	-51.6	3.3
HT3	Virtual step	-9.1	-6.0	-0.7	-51.7	3.6
OrthHT1	Virtual step	-1.9	-9.1	-0.7	-61.1	3.3
HexHT1	Virtual step	3.6	-6.0	-3.6	-19.9	3.5
DinuHT1	Virtual step	-3.0	4.8	-0.6	-48.5	3.7

Supplementary Table 3.

Base pair parameters of various helices under comparison

Sequence	**Base pair**	**Tip** (°)	**Incl** (°)	**Prop** (°)	**Buck** (°)	**Xdisp** **(Å)**
CGCGCG	C1.G12	6.3	-5.6	-0.2	-2.8	3.0
HT5	C1.G12	3.6	-16.2	-3.1	3.2	2.4
HT3	C1.G12	8.8	4.8	5.4	-0.2	5.8
OrthHT1	T1.A12	2.8	-9.7	9.2	6.3	3.0
HexHT1	T1.A12	3.6	-6.7	5.5	3.2	3.3
CGCGCG	G2.C11	2.0	-4.2	-3.9	4.4	2.6
HT5	G2.C11	-3.5	-15.6	-2.0	-8.5	2.8
HT3	G2.C11	-11.6	10.5	-6.3	-7.0	4.5
OrthHT1	G2.C11	-1.7	-4.8	-3.0	-5.5	2.1
HexHT1	G2.C11	-9.8	-6.5	6.1	6.1	2.6
CGCGCG	C3.G10	1.2	-2.7	-1.8	-4.5	1.6
HT5	C3.G10	13.0	-7.3	2.1	8.2	2.7
HT3	T3.A10	10.4	9.8	5.3	2.6	4.5
OrthHT1	C3.G10	3.1	-2.8	-2.0	2.7	0.9
HexHT1	C3.G10	2.0	-2.4	7.4	4.7	1.2
CGCGCG	G4.C9	-2.3	-3.7	-0.1	4.5	1.6
HT5	G4.C9	9.7	-6.5	0.5	-7.4	2.3
HT3	G4.C9	6.1	12.1	-2.4	11.1	4.3
OrthHT1	G4.C9	-0.6	-2.7	0.4	-6.0	0.8
HexHT1	G4.C9	2.6	-2.0	0.6	7.3	1.1
CGCGCG	C5.G8	-0.4	-4.4	-0.7	-3.3	2.7
HT5	T5.A8	8.5	2.8	-1.8	5.6	3.2
HT3	C5.G8	-7.8	7.5	-6.1	-0.1	4.9
OrthHT1	C5.G8	-0.6	-3.3	-3.0	-0.9	2.1
HexHT1	C5.G8	-2.3	-2.7	2.5	0.4	2.1
DinuHT1	T13.G16	0.8	-6.9	8.3	4.8	3.3

CGCGCG	G6.C7	-1.7	-5.3	2.4	0.1	3.1
HT5	G6.C7	4.9	2.4	-0.1	-3.2	3.3
HT3	G6.C7	-3.0	7.6	7.5	6.1	5.0
OrthHT1	G6.C7	-0.1	-5.4	6.7	-4.8	2.6
HexHT1	G6.C7	-2.4	-5.1	5.7	5.9	2.9
DinuHT1	G16.T15	2.6	-6.6	-0.5	-6.4	3.5

Supplementary Table 4:

Backbone torsions angles of the helices under comparison

Sequence	**Base**	α (°)	β (°)	γ (°)	δ (°)	ε (°)	ζ (°)	χ (°)	**P** (°)
Strand 1									
CGCGCG	C1	-	-	52.4	144.9	265.4	78.9	209.5	154.1
HT5	C1	-	-	57.1	134.0	274.5	69.2	208.3	145.0
HT3	C1	-	-	224.0	161.5	114.9	220.8	212.5	204.1
OrthHT1	T1	-	-	56.1	140.1	266.4	74.1	208.5	164.3
HexHT1	T1	-	-	52.7	146.0	260.5	76.6	214.3	169.7
DinuHT1	T13	-	-	237.6	61.3	141.9	262.5	209.9	159.2
CGCGCG	G2	61.5	187.7	178.5	90.9	239.9	294.7	60.3	40.0
HT5	G2	72.5	193.0	174.6	98.8	239.1	318.0	65.4	63.0
HT3	G2	62.9	222.2	234.0	137.6	224.9	359.2	70.3	233.9
OrthHT1	G2	85.1	190.3	162.3	89.7	232.0	306.7	65.6	50.0
HexHT1	G2	66.5	185.6	179.5	101.4	241.6	304.5	54.2	38.1
DinuHT1	G14	70.6	65.2	179.5	189.9	-	-	79.0	136.7
CGCGCG	C3	212.7	239.0	50.1	148.1	260.1	81.0	209.7	145.3
HT5	C3	212.0	206.5	42.9	145.9	266.6	72.5	213.9	167.8
HT3	T3	295.1	189.0	294.1	156.7	245.1	93.4	200.5	182.3
OrthHT1	C3	198.7	229.2	60.8	145.2	263.8	77.5	209.3	161.0
HexHT1	C3	194.2	212.4	72.3	143.0	259.9	71.4	212.1	156.6
CGCGCG	G4	64.4	186.3	179.5	91.8	181.1	69.3	58.6	25.9
HT5	G4	69.7	189.7	169.6	86.5	244.1	290.8	64.8	36.8
HT3	G4	101.6	191.0	167.0	104.7	206.9	342.3	50.7	73.3
OrthHT1	G4	65.8	187.7	180.1	99.0	184.2	60.2	59.1	29.8
HexHT1	G4	68.2	180.1	174.1	105.8	245.9	298.7	60.3	30.0
CGCGCG	C5	166.4	159.9	48.3	141.9	260.1	79.7	208.0	150.8
HT5	T5	194.7	230.5	61.9	127.5	257.1	80.7	207.8	150.6
HT3	C5	146.6	201.7	91.4	123.2	243.5	112.3	195.9	136.4
OrthHT1	C5	156.0	155.0	59.3	141.6	263.7	74.9	210.6	150.4
HexHT1	C5	194.5	223.7	62.5	147.4	263.9	62.5	223.6	166.3
CGCGCG	G6	76.5	175.4	182.3	148.8	-	-	78.1	170.1
HT5	G6	75.0	171.9	185.4	150.6	-	-	73.3	172.0
HT3	G6	31.6	197.3	201.9	127.4	-	-	60.8	194.9
OrthHT1	G6	81.9	179.8	182.7	147.5	-	-	75.7	170.6
HexHT1	G6	80.6	178.5	190.8	138.1	-	-	71.5	168.9

Strand 2									
Sequence	**Base**	α (°)	β (°)	γ (°)	δ (°)	ε (°)	ζ (°)	χ (°)	**P** (°)
CGCGCG	C7	-	-	54.7	139.1	267.8	74.0	209.3	156.7
HT5	C7	-	-	21.5	155.5	274.9	49.9	223.2	189.7
HT3	C7	-	-	263.7	167.3	207.2	192.1	177.4	199.3
OrthHT1	C7	-	-	57.2	142.9	262.8	78.5	202.9	157.0
HexHT1	C7	-	-	45.1	147.8	274.9	65.9	219.2	166.2
DinuHT1	T15	-	-	173.1	54.1	141.1	261.1	203.7	153.0
CGCGCG	G8	67.1	188.7	172.4	101.0	236.4	335.2	61.3	36.2
HT5	A8	98.7	180.6	163.2	93.7	232.4	305.5	63.0	49.2
HT3	G8	231.2	123.0	81.7	89.3	178.5	63.0	57.4	77.4
OrthHT1	G8	65.3	187.8	179.4	95.4	176.5	63.3	62.1	27.5
HexHT1	G8	68.7	174.6	184.6	106.0	237.9	310.2	62.7	38.2
DinuHT1	G16	75.6	60.8	188.0	183.2	-	-	58.3	19.8
CGCGCG	C9	198.1	196.4	55.1	140.0	268.4	73.8	205.7	152.9
HT5	C9	179.7	223.3	72.1	139.0	270.8	67.2	205.6	151.4
HT3	C9	257.3	163.0	315.4	155.3	239.9	86.8	242.9	191.7
OrthHT1	C9	160.5	157.1	59.5	142.7	261.8	74.6	207.6	160.2
HexHT1	C9	199.3	223.6	52.5	146.8	270.2	68.5	226.6	165.0
CGCGCG	G10	64.3	185.4	178.9	96.0	244.3	290.2	62.1	35.2
HT5	G10	95.0	183.6	151.1	81.2	228.3	316.3	61.9	41.0
HT3	A10	63.1	151.1	175.0	120.8	275.7	283.0	71.5	-73.3
OrthHT1	G10	70.0	185.5	176.7	97.9	257.7	291.8	58.4	16.3
HexHT1	G10	69.1	179.2	181.4	105.2	230.2	329.5	59.9	53.9
CGCGCG	C11	209.8	240.7	56.3	142.2	258.8	70.2	203.7	150.8
HT5	C11	208.4	211.3	52.7	139.5	253.8	71.0	203.8	149.7
HT3	C11	348.4	171.1	304.6	152.1	64.2	293.8	196.1	191.8
OrthHT1	C11	200.6	224.1	67.2	136.8	259.3	69.0	210.3	156.2
HexHT1	C11	198.2	204.3	50.1	151.7	272.8	59.6	221.3	166.0
CGCGCG	G12	84.3	183.0	182.9	148.8	-	-	72.5	161.9
HT5	G12	87.8	173.4	179.1	144.9	-	-	76.3	170.6
HT3	G12	282.9	160.3	51.4	70.6	-	-	50.4	56.4
OrthHT1	A12	77.1	181.6	192.4	147.2	-	-	67.6	171.1
HexHT1	A12	91.6	170.5	185.8	142.2	-	-	69.1	164.7