

## RNA

ar0001 2.30  
ar0002 2.50  
ar0004 2.50  
ar0006 1.90  
ar0008 2.10  
ar0009 1.16  
ar0010 1.40  
ar0011 2.50  
ar0012 1.60  
ar0013 1.16  
ar0014 1.23  
ar0019 0.97  
ar0020 1.20  
ar0022 1.90  
ar0023 1.60  
ar0025 2.10  
ar0028 2.10  
ar0029 1.70  
ar0032 2.18  
ar0033 1.80  
ar0034 1.40  
arh064 1.80  
arh074 1.46  
arl048 1.80  
arl062 2.60  
arn035 2.25  
ur0001 2.70  
ur0005 2.30  
ur0025 2.50  
url029 2.64  
url050 2.40  
url064 1.50  
urx063 2.40

## DNA

bd0001 1.60  
bd0002 2.70  
bd0003 2.80  
bd0004 3.0  
bd0005 1.75  
bd0006 1.15  
bd0007 1.1  
bd0008 1.43  
bd0009 1.6  
bd0010 2.0  
bd0011 2.3  
bd0015 2.5  
bd0019 1.70

bd0022 2.6  
bd0023 0.74  
bd0024 1.20  
bd0025 1.50  
bd0027 1.60  
bd0028 2.50  
bd0029 1.82  
bd0031 1.60  
bdj008 1.30  
bdj017 1.60  
bdj019 1.40  
bdj025 1.50  
bdj031 1.50  
bdj036 1.70  
bdj037 2.00  
bdj039 2.20  
bdj051 2.00  
bdj052 1.90  
bdjb44 1.30  
bdjb48 2.00  
bdjb49 1.70  
bdjb50 1.70  
bdjb57 1.60  
bdjb77 2.50  
bdl084 1.40  
bdlb03 3.00  
bdlb04 2.30  
bdlb10 2.50  
bdlb13 2.00  
bdlb26 2.00  
bdlb33 2.80  
bdlb04 2.30  
bdlb40 2.40  
bdlb53 2.90  
bdlb54 2.250  
bdlb56 2.50  
bdlb58 2.250  
bdlb72 2.01  
bdlb73 2.03  
bdlb74 2.01  
bdlb76 2.50  
bdlb82 2.50  
bdlb83 2.70  
bdlb84 1.55  
bdlb85 1.55  
bdls67 2.40  
bdls79 2.50  
bdls80 2.14  
dd0020 2.27  
udj031 2.50

udj048 2.60  
udj049 2.00  
udj060 2.60

**Table S1.** NDB code of the structures of RNA and DNA used in this study. The resolution of the crystal is indicated.

## B-DNA

Step	N	Shift	Slide	Rise	Tilt	Roll	Twist
AA	55	-0.06(0.3)	-0.16(0.4)	3.28(0.1)	0.1(2)	1.4(5)	35(4)
AC	18	0.06(0.6)	-0.43(0.3)	3.23(0.2)	-0.3(2)	1.4(4)	32(2)
AG	10	0.06(0.4)	0.34(0.4)	3.27(0.1)	0.2(3)	5.5(4)	28(6)
AT	44	0.12(0.3)	-0.57(0.2)	3.30(0.1)	0.3(3)	-1.2(3)	31(4)
CA	32	0.02(0.3)	1.88(1.0)	3.32(0.2)	0.0(3)	-1.2(6)	43(9)
CC	21	0.05(0.6)	0.28(0.3)	3.40(0.2)	-0.1(3)	3.9(4)	35(4)
CG	64	0.06(0.5)	0.68(0.3)	3.25(0.2)	0.0(3)	6.2(3)	31(6)
GA	47	0.00(0.5)	-0.01(0.4)	3.43(0.1)	0.0(3)	0.4(4)	41(4)
GC	67	-0.30(0.8)	0.31(0.4)	3.57(0.2)	0.0(5)	-6.8(5)	40(4)
TA	9	-0.17(0.3)	0.38(0.7)	3.37(0.2)	-1.4(2)	-0.6(4)	43(5)
Total	367	-0.03(0.6)	0.26(0.8)	3.36(0.2)	0.0(3)	0.3(6)	36(7)

## A-RNA

Step	N	Shift	Slide	Rise	Tilt	Roll	Twist
AA	9	-0.08(0.3)	-1.27(0.4)	3.18(0.2)	-0.8(2)	7.0(3)	31(5)
AC	17	0.23(0.5)	-1.43(0.3)	3.24(0.2)	0.8(4)	4.8(3)	32(3)
AG	30	-0.04(0.5)	-1.50(0.3)	3.30(0.1)	0.5(2)	8.5(3)	30(2)
AU	8	-0.06(0.3)	-1.36(0.3)	3.24(0.2)	1.1(2)	7.1(4)	33(4)
CA	25	0.11(0.5)	-1.46(0.2)	3.09(0.2)	1.0(2)	9.9(3)	31(3)
CC	41	-0.01(0.5)	-1.78(0.3)	3.32(0.2)	0.3(4)	8.7(4)	32(3)
CG	18	0.30(0.4)	-1.89(0.4)	3.30(0.3)	-0.1(2)	12.1(6)	27(4)
GA	13	0.07(0.5)	-1.70(0.5)	3.38(0.3)	1.3(4)	9.4(4)	32(4)
GC	28	0.07(0.6)	-1.39(0.2)	3.22(0.1)	0.0(3)	6.1(3)	35(4)
UA	30	-0.02(0.4)	-1.45(0.2)	3.26(0.2)	-0.2(3)	10.7(3)	32(4)
Total	209	0.05(0.5)	-1.56(0.3)	3.26(0.2)	0.4(3)	8.6(4)	32(4)

**Table S2.** Mean helical parameters (standard deviations in parenthesis) for the 10 different B-DNA and A-RNA steps in the database. Translational and rotational parameters are in Å and degrees. Total values correspond to the averages determined for all the structures in the database.