

Supplemental Methods.

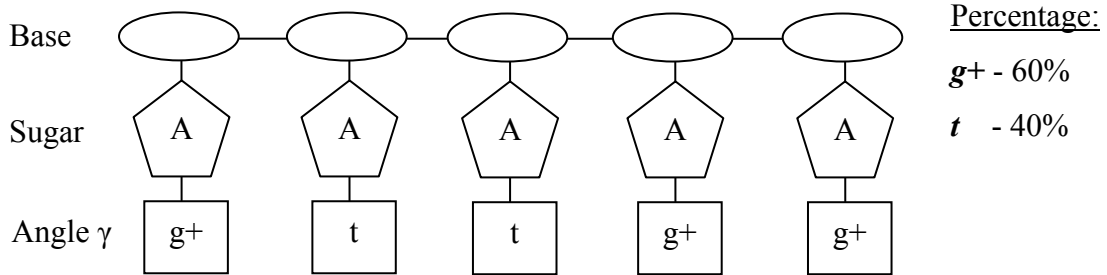
Calculation of the quantity of DNA fragments having the same percentage of nucleotides with alternative angle γ conformations among nucleotides with A or B-like sugar pucker (Table 3) in the paper).

The data has been obtained after the following sequence of calculations:

- determine the sugar pucker and angle γ conformation in each nucleotide in all DNA fragments,
- calculate the percentage of nucleotides in each angle γ conformations among all A-like and B-like nucleotides in each DNA fragment,
- calculate the quantity of DNA fragments having the same percentage of nucleotides with alternative angle γ conformations among nucleotides with A or B-like sugar pucker,
- add the value into the table.

Below are 3 examples of a naked A-DNA and B-DNA fragments and a bound oligonucleotide.

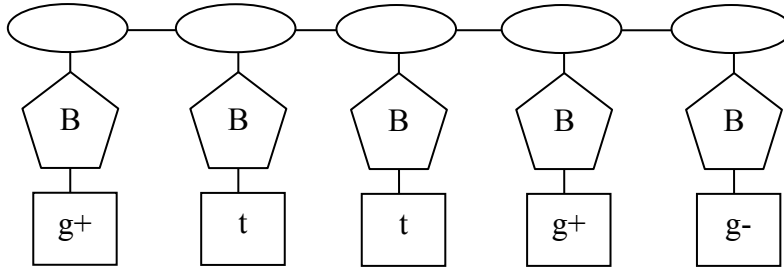
a) Naked A-DNA



The input of this fragment to the table is as follows:

		Naked DNA				Bound DNA			
N		A-like		B-like		A-like		B-like	
N1									
P	γ angle	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>
		0 %							
	1 – 10 %								
	11 – 20 %								
	21 – 30 %								
	31 – 40 %	1							
	41 – 50 %								
	51 – 60 %								
	61 – 70 %								
	71 – 80 %								
	81 – 90 %								
	91 – 100 %								

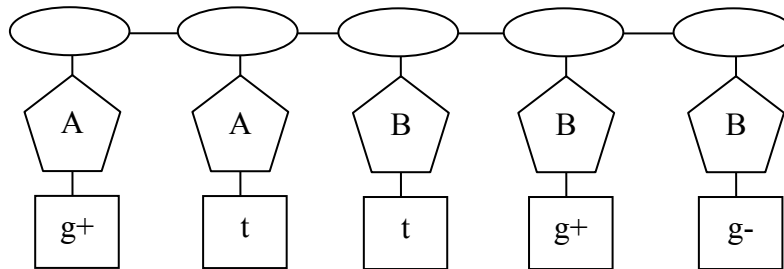
b) Naked B-DNA



Percentage
g+ - 40%
t - 40%
g- - 20%
t & g- - 60%

		Naked DNA				Bound DNA			
N									
		A-like		B-like		A-like		B-like	
N1									
P	γ angle	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>
		0 %							
	1 - 10 %								
	11 - 20 %			1					
	21 - 30 %								
	31 - 40 %		1						
	41 - 50 %								
	51 - 60 %				1				
	61 - 70 %								
	71 - 80 %								
	81 - 90 %								
	91 - 100 %								

c) Bound DNA



Percentage:
 A-like
g+ - 50%
t - 50%
 B-like
g+ - 33%
g- - 33%
t & g- - 66%

		Naked DNA				Bound DNA			
N									
		A-like		B-like		A-like		B-like	
N1									
P	γ angle	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>	<i>t</i>	<i>t</i>	<i>g-</i>	<i>t & g-</i>
		0 %							
	1 - 10 %								
	11 - 20 %								
	21 - 30 %								
	31 - 40 %					1	1		

41 – 50 %					1			
51 – 60 %								
61 – 70 %								1
71 – 80 %								
81 – 90 %								
91 – 100 %								

Supplemental tables

Supplemental Table 1. PDB IDs of structures included in the study

Naked A-DNA	118D 137D 138D 160D 1D78 1D79 1DNZ 1M77 1VJ4 1VT8 1XJX 1Z7I 1ZEX 1ZEY 1ZF1 1ZF6 1ZF8 1ZFA 212D 213D 243D 260D 295D 2A7E 2D94 2HC7 2PKV 2PL4 317D 338D 344D 345D 348D 349D 368D 369D 370D 371D 395D 396D 399D 414D 440D 9DNA
Naked B-DNA	122D 423D 428D 431D 436D 460D 461D 463D 476D 477D 1D8G 1DOU 1DPN 1EHV 1EN3 1EN8 1EN9 1ENE 1ENN 1EI4 1FQ2 1G8U 1G8V 1IKK 1JGR 1S23 1S2R 1SK5 1ZF0 1ZF5 1ZF7 1ZFB 1ZFG 1ZFF 2QEG 251D 1BD1 5DNB 1D23 1D49 1D56 158D 196D 307D 1BNA 7BNA 9BNA 355D
Protein-DNA complexes	1AAAY 1AZP 1BF4 1CDW 1CKQ 1D02 1DC1 1DFM 1DP7 1DSZ 1E3O 1EGW 1ESG 1FIU 1GU4 1H6F 1JX4 1L1Z 1L3L 1LLM 1LMB 1M5R 1MNN 1MUS 1NKP 1ORN 1QNA 1QUM 1RH6 1SX5 1TDZ 1TRO 1WTE 1XYI 1ZS4 2A07 2BOP 2C7P 2E42 2EA0 2FMP 2G1P 2HOS 2IH2 2NQ9 2O4A 2OAA 2ODI 2OFI 2PFN 2R1J 2VBO 2VE9 2VLA 2VOA 2W42 2W7N 2WBS 2WIW 2XHI 2XO6 3AAF 3BAM 3BM3 3BS1 3DVO 3E6C 3FDE 3FDQ 3FSI 3G00 3G9M 3GOX 3HTS 3I0W 3I8D 3IGK 3JXY 3KDE 3KXT 3L2C 3M4A 3MR3 3NDH 3O1P 3OQG 3OSN 3PV8 3PVI 3QMD 3RKQ 3SAU 3SM4 3SQ1 3V6T

Supplemental Table 2. Percentages of nucleotides with different conformations of the torsion angle γ in the naked A-DNA, naked B-DNA and DNA that form complexes with proteins in the dataset of structure with a resolution better than 1.5 Å. The dataset contain the 15 and 22 structures of naked A- and B-DNA, and 15 oligonucleotides from complexes with proteins. Total number of nucleotides is 629.

Sugar pucker	Naked DNA			Bound DNA		
	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>
A-like	87.3	0	12.7	57.4	0	42.6
B-like	100.0	0	0	95.5	1.3	3.2

Supplemental Table 3. Standard deviation of the absolute values of the ASA (Å²) of the polar and hydrophobic atoms exposed in the minor and major grooves in nucleotides with the two types of sugar pucker in DNA bound to proteins.

Entire Surface										
	A-like nucleotides				B- like nucleotides					
	Major groove		Minor groove		Major groove			Minor groove		
	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>
Polar ASA										
mean	10.3	10.9	6.8	10.8	7.1	8.5	14.2	8.1	5.8	15.8
Adenine	10.4	8.1	6.9	9.1	5.4	4.7	19.9	5.5	4.2	18.1
Cytosine	5.7	4.9	5.6	6.0	5.9	3.9	9.4	6.3	3.9	8.7
Guanine	10.6	13.2	5.7	14.5	6.2	12.7	16.7	7.5	7.4	20.3
Thymine	7.1	8.5	8.2	8.3	5.8	3.2	5.1	6.4	5.1	6.3
Hydrophobic ASA										
mean	12.4	16.6	8.9	8.7	16.5	24.8	18.6	7.2	5.0	11.8
Adenine	5.5	7.3	11.6	8.3	9.2	7.9	14.9	7.3	4.3	19.5
Cytosine	8.2	8.0	5.5	6.4	11.6	7.5	18.0	5.7	3.5	7.3
Guanine	5.7	12.4	9.0	9.4	8.9	28.9	11.2	6.2	4.1	9.9
Thymine	9.3	13.0	6.3	6.2	11.7	9.8	11.4	5.8	3.0	7.9
Sugar-phosphate backbone										
	A-like nucleotides				B- like nucleotides					
	Major groove		Minor groove		Major groove			Minor groove		
	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>
Polar ASA										
mean	5.2	6.5	5.4	8.1	5.9	3.9	11.4	5.8	4.6	12.4
Adenine	5.0	5.6	6.0	9.1	5.7	3.7	18.3	5.7	4.1	16.9
Cytosine	3.3	4.4	4.3	5.2	6.3	4.6	7.9	6.2	3.5	8.1
Guanine	5.7	8.4	5.6	9.7	5.7	3.1	10.4	5.4	5.7	12.6
Thymine	5.6	5.3	6.3	6.1	5.7	3.5	5.1	5.9	4.2	4.5
Hydrophobic ASA										
mean	1.8	5.9	6.2	7.8	4.6	5.6	10.4	6.1	4.8	10.4
Adenine	2.5	5.0	7.9	7.6	4.4	4.1	11.1	6.2	3.6	16.9
Cytosine	1.7	4.9	5.1	6.3	5.2	3.9	12.5	5.7	3.5	7.1
Guanine	1.9	7.1	6.7	8.7	4.5	11.9	8.5	5.8	10.1	9.0
Thymine	1.4	4.0	5.4	6.2	4.5	3.8	6.9	5.7	3.0	7.9
Bases										
	A-like nucleotides				B- like nucleotides					
	Major groove		Minor groove		Major groove			Minor groove		
	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>
Polar ASA										
mean	7.4	8.1	5.1	4.7	5.6	8.6	6.7	5.6	5.7	6.5
Adenine	7.3	5.5	3.1	1.0	4.7	4.9	4.5	1.8	1.2	1.9
Cytosine	4.4	3.7	3.0	1.9	3.8	2.8	5.7	2.1	1.8	2.7
Guanine	8.0	8.6	5.9	6.3	4.9	11.8	7.4	5.9	2.7	9.1
Thymine	5.2	3.5	6.2	2.3	2.6	2.2	2.3	2.8	2.7	3.4

Hydrophobic ASA										
mean	12.0	14.6	4.2	2.6	14.7	23.0	13.4	2.9	3.3	3.6
Adenine	3.9	3.8	4.6	2.3	5.5	3.9	4.5	3.2	1.8	3.2
Cytosine	7.2	4.1	1.5	0.8	6.9	4.4	7.1	0.4	0.0	2.2
Guanine	4.8	6.5	3.8	2.4	4.8	17.1	3.4	1.6	6.4	4.2
Thymine	8.8	9.2	1.4	0.0	8.1	6.5	5.1	0.6	0.0	0.0

Supplemental Table 4. Standard deviation of the mean values of the ASA (\AA^2) of the O3', O5' and C5' atoms in nucleotides with the A-like and B-like sugar pucker and different γ angle conformations in the minor and major grooves.

	A-like nucleotides				B-like nucleotides					
	Major		Minor		Major			Minor		
γ angle	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>	<i>g</i> ⁺	<i>g</i> ⁻	<i>t</i>
O3'										
mean	1.3	0.9	1.3	1.1	0.1	0.0	0.1	1.7	1.4	1.6
Adenine	0.8	1.3	1.1	1.5	0.1	0.0	0.1	1.6	1.1	2.3
Cytosine	1.8	1.3	1.3	1.3	0.1	0.0	0.2	1.9	2.1	0.9
Guanine	1.7	0.0	1.4	0.6	0.2	0.0	0.0	1.8	1.2	1.3
Thymine	1.3	0.0	1.2	0.7	0.0	0.0	0.0	1.7	0.7	1.3
O5'										
mean	0.9	1.4	0.1	3.2	0.7	1.5	1.6	0.2	1.4	3.2
Adenine	0.4	1.3	0.2	2.7	0.8	1.2	2.0	0.1	1.0	4.0
Cytosine	1.1	0.1	0.1	2.2	0.7	1.9	1.6	0.2	1.2	3.1
Guanine	1.1	2.1	0.2	3.0	0.8	0.7	0.9	0.3	1.6	3.1
Thymine	0.6	0.1	0.1	2.6	0.4	1.0	1.6	0.1	1.3	3.1
C5'										
mean	0.2	5.3	2.4	2.9	0.2	2.5	8.1	2.7	2.8	4.8
Adenine	0.2	4.6	2.5	3.3	0.2	1.7	10.7	2.9	1.9	7.5
Cytosine	0.2	3.5	2.5	2.4	0.3	1.4	7.0	2.3	2.0	2.7
Guanine	0.3	6.7	2.7	2.9	0.2	6.0	7.2	2.8	4.8	3.5
Thymine	0.1	3.1	1.5	2.2	0.1	1.2	7.2	2.4	1.8	3.0