DNA curvature, melting, and flexibility

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Comparative Microbial Genomics Workshop
Pathumthani, Thailand
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Outline

- Introduction & disclaimer
- DNA curvature
- DNA Flexibility
360° = one helical turn
10.5 bp per turn
34.3° twist angle (rotation per residue)

Helix Pitch
35.7 Å

Helix Diameter
20 Å

Major Groove

Base Pair Tilt - 6°

Minor Groove

3.4 Å Axial Rise
2.1

200 bp

A. Straight DNA

200 bp

Bent DNA

B.
**Figure 8.10** Electron micrograph of a portion of a 2% agarose gel, 1 \( \mu \text{m} \times 0.5 \mu \text{m} \) overall: small black rectangle is 1000 Å \( \times \) 500 Å. Individual gel fibers are about 100 Å wide. Courtesy of Sue Whytock and John Finch.
Random Bends

Bends Phased at 10.5 bp

Bends Phased at 16 bp
Intrinsic Curvature
dev  avg
0.07  0.30
Stacking Energy
dev  avg
-9.52 -6.40
Position Preference
dev  avg
0.11  0.17
Annotations:
- CDS +
- CDS -
Direct Repeats
fix  avg
5.00  7.50
Inverted Repeats
fix  avg
5.00  7.50
Percent AT
fix  avg
0.30  0.70
Resolution: 19

E. coli  pO157
GenBank Accession AF074613  92,077 bp
Escherichia coli K-12, isolate MG1655

4,639,221 bp
Promoter Structural profile

“UP” -35 -10 “TATA box”
**Ecoli_K−12_W3110_Main**

**CURVATURE**

The graph shows the stacking energy of the sequence Ecoli_K−12_W3110_Main as a function of distance from the translation start. The x-axis represents the distance from the translation start, ranging from -400 to 400, while the y-axis represents the Z-score, ranging from -0.05 to 0.25. The red line indicates the stacking energy curve, with significant peaks and troughs indicating areas of high and low stacking energy, respectively.
Promoter Structural profile

DNA curvature, flexibility important here

CDS

CDS

mRNA

cruciform

rigid melts

-35

-10

+1

β / β'

α
2.10
"Refined" Junction Model

CGG
Tilt
CGGC
5' 3'

GGCC GCCG

A
T
5' 3'

A A A AA
T
T

Roll
+
Tilt

3' 5'

T TT
A
T
A
T
A
T
A
T
A
T
A
T
A
T
A
T
A
T

2.11

5'3' 5' 3'
Histones H2A, H2B, H3, H4 (two molecules each)

Nucleosome

Linker DNA

Core DNA

Internal structure

55 Å

110 Å
(B) Chromatin in form of “beads on a string”

![Diagram showing chromatin structure with beads on a string and light nuclease digestion.]

Light nuclease digestion

Average length of DNA fragment ~200 bp per nucleosome
Light nuclease digestion

Average length of DNA fragment ~200 bp per nucleosome

Heavier nuclease digestion

Average length of core DNA ~145 bp per core particle
“Travers” trinucleotide scale:


NOTE: we use a (slight) modification, in which the absolute value (magnitude) of the values is used to reflect trinucleotides which tend to exclude nucleosomes.

Schizosaccharomyces pombe

All Three Chromosomes  11,896,623 bp total

Schizosaccharomyces pombe
strain 972, chromosome I   5,570,797 bp

A) Intrinsic Curvature
B) Stacking Energy
C) Position Preference
D) Annotations:
   - CDS +
   - CDS -
   - rRNA
   - tRNA
E) Global Direct Repeats
F) Global Inverted Repeats
G) GC Skew
H) Percent AT
Schizosaccharomyces pombe

strain 972, chromosome I  5,570,797 bp

Resolution: 2
Figure 7. Structural cluster analysis. Distance tree showing the relative location of 11 gene clusters based on average structural measures. The number of genes in
Highly Expressed Genes
Summary

1. DNA sequence ➞ DNA structure ➞ Function

2. DNA curvature is caused mainly by phased A-tracts.

3. Where you are in the chromosome is important!