Mesoscale Simulations of Two Nucleosome-Repeat Length Oligonucleosomes

Supplemental figures

[Submitted to the Special Issue of *Physical Chemistry Chemical Physics*,
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Figure captions

Figure S1: Nucleosome contact patterns for 12-unit oligonucleosomes at two nucleosome repeat lengths (NRL) at 0.15 monovalent salt, with and without linker histone (+/−LH), and with and without divalent ions (+/−Mg), from zigzag (dashed) and solenoid (solid line) starting configurations.

Figure S2: DNA bending angle distributions for for 12-unit oligonucleosomes at the longer repeat length (NRL = 209) at 0.15 monovalent salt, with and without linker histone (+/−LH), and with and without divalent ions (+/−Mg), from zigzag (dashed) and solenoid (solid line) starting configurations.

Figure S3: Convergence of the Monte Carlo sampling accessed through the behavior of the total fiber energy, sedimentation coefficients, triplet angles, and dimer distances between three consecutive nucleosomes, with linker histone and monovalent salt, averaged over 12 simulations started from zigzag (a) and solenoid (b) initial configurations (24-mer oligonucleosomes).

Figure S4: Total energy, triplet angles (cumulative average), and dimer distances (cumulative average) for three different trajectories for zigzag (a), and solenoid (b) starting configurations.

Figure S5: Description of the fiber axis calculation for 24-unit oligonucleosome. a) Cyan - nucleosome cores, Red lines - connections between consecutive nucleosomes, Green line - fiber axis, as estimated by the least squares procedure; b) Fiber axis decomposition into three separate curves for three vectors (x, y, and z); Blue dots - nucleosome centers, Green line - fiber axis, Red dots - separators between line segments of the fiber axis.

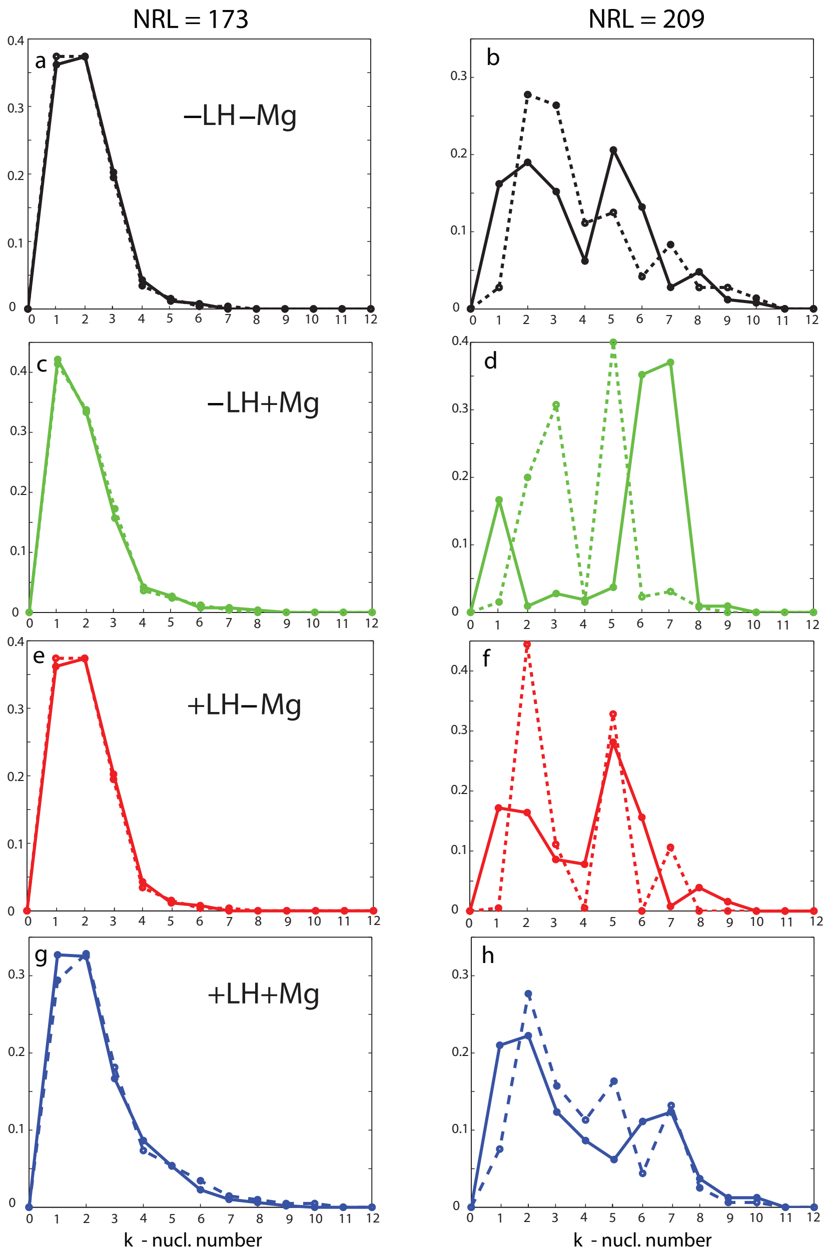
NRL = 173
NRL = 209
a
b
c
d
e
f
g
h
−LH−Mg
−LH+Mg
+LH−Mg
+LH+Mg
0
0.1
0.2
0.3
0.4
0 1 2 3 4 5 6 7 8 9 10 11 12
k - nucl. number
k - nucl. number

Figure S1:

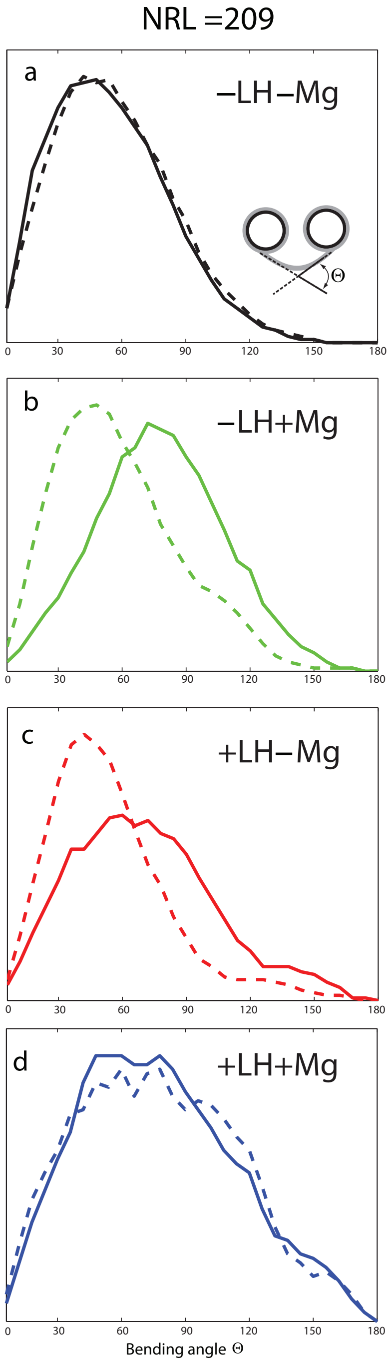
NRL =209
a
−LH−Mg
Θ
0
30
60
90
120
150
180
b
−LH+Mg
0
30
60
90
120
150
180
c
+LH−Mg
0
30
60
90
120
150
180
d
+LH+Mg
0
30
60
90
120
150
180
Bending angle Θ

Figure S2:

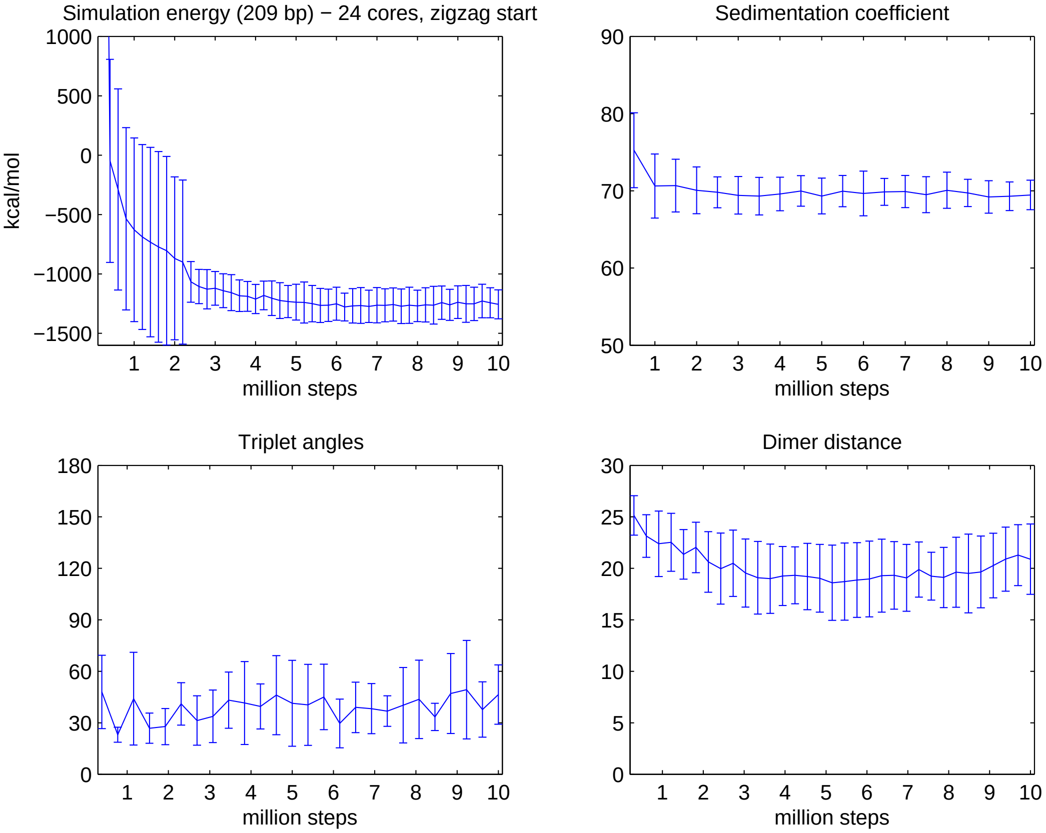
Simulation energy (209 bp) − 24 cores, zigzag start
kcal/mol
1000
500
0
−500
−1000
−1500
1 2 3 4 5 6 7 8 9 10
million steps
Sedimentation coefficient
90
80
70
60
50
1 2 3 4 5 6 7 8 9 10
million steps
Triplet angles
180
150
120
90
60
30
0
1 2 3 4 5 6 7 8 9 10
million steps
Dimer distance
30
25
20
15
10
5
0
1 2 3 4 5 6 7 8 9 10
million steps

Figure S3:

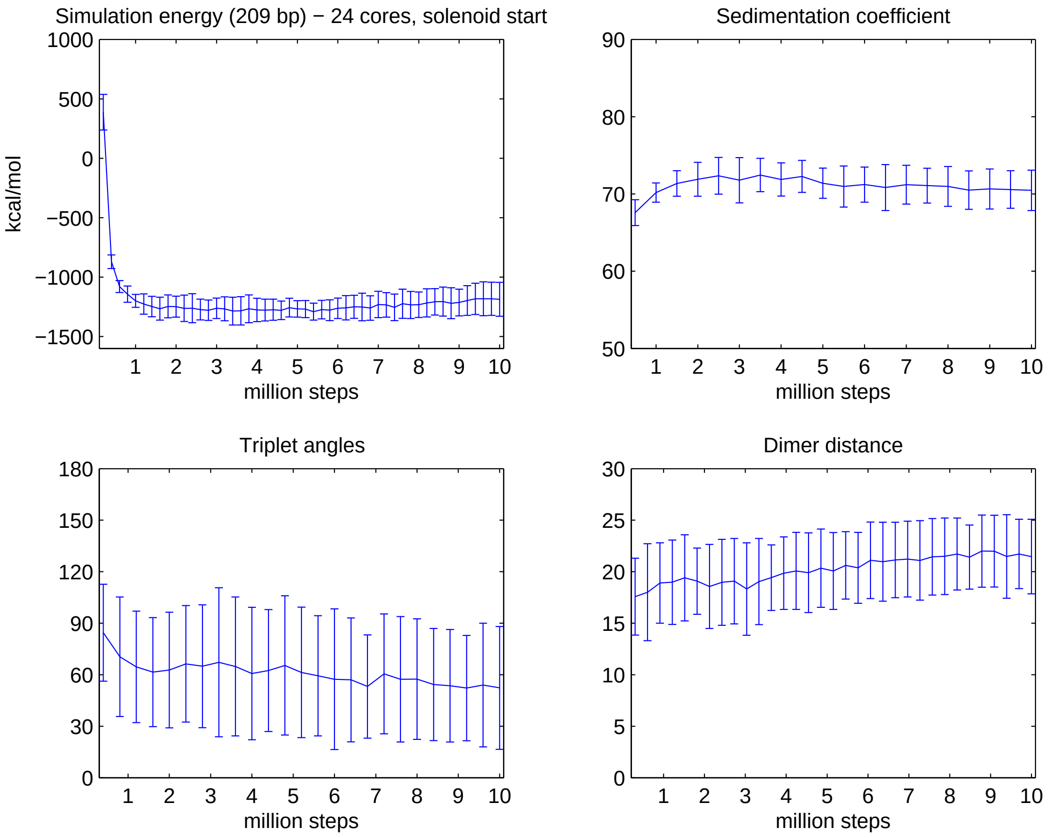

Figure S3: cont.

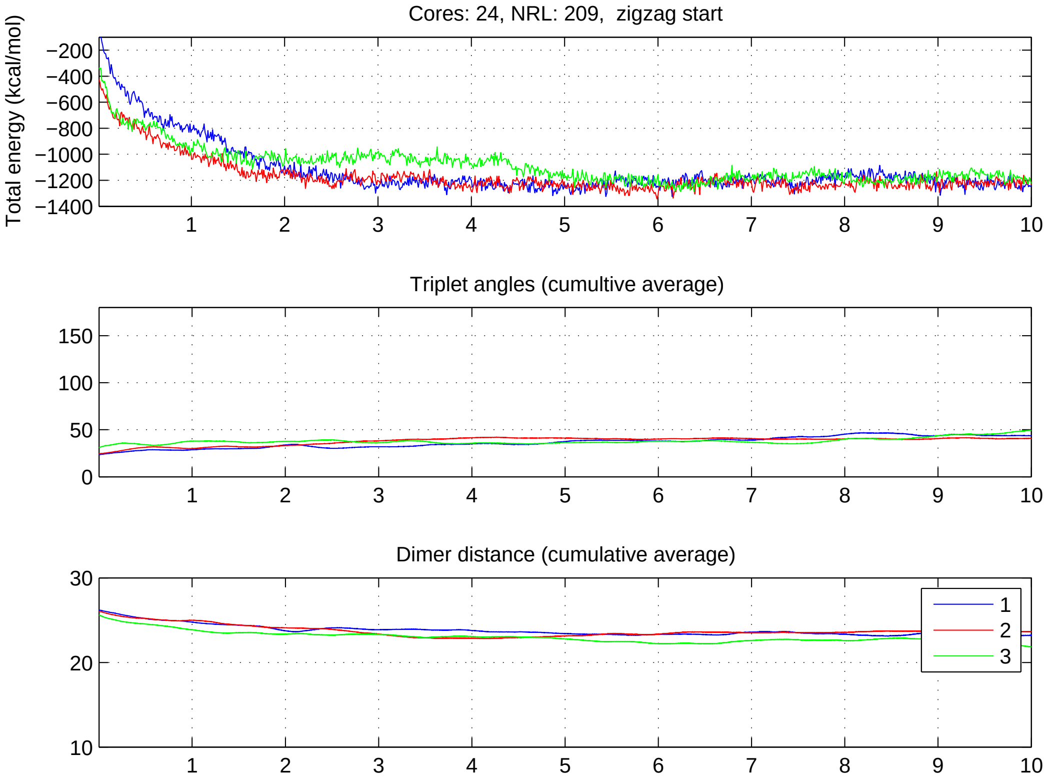
Cores: 24, NRL: 209, zigzag start
Total energy (kcal/mol)
−200
−400
−600
−800
−1000
−1200
−1400
1
2
3
4
5
6
7
8
9
10
Triplet angles (cumultive average)
150
100
50
0
Dimer distance (cumulative average)
30
20
10
1
2
3

Figure S4: a

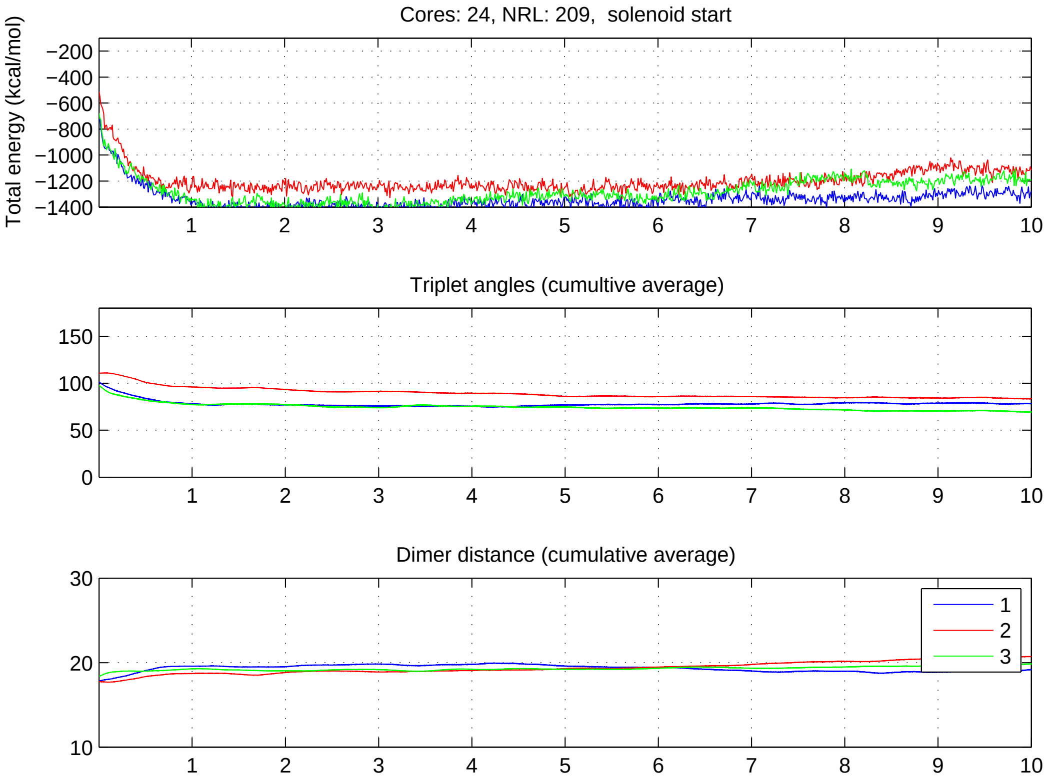
Cores: 24, NRL: 209, solenoid start
Total energy (kcal/mol)
−200
−400
−600
−800
−1000
−1200
−1400
1
2
3
4
5
6
7
8
9
10
Triplet angles (cumultive average)
150
100
50
0
Dimer distance (cumulative average)
30
20
10
1
2
3

Figure S4: b

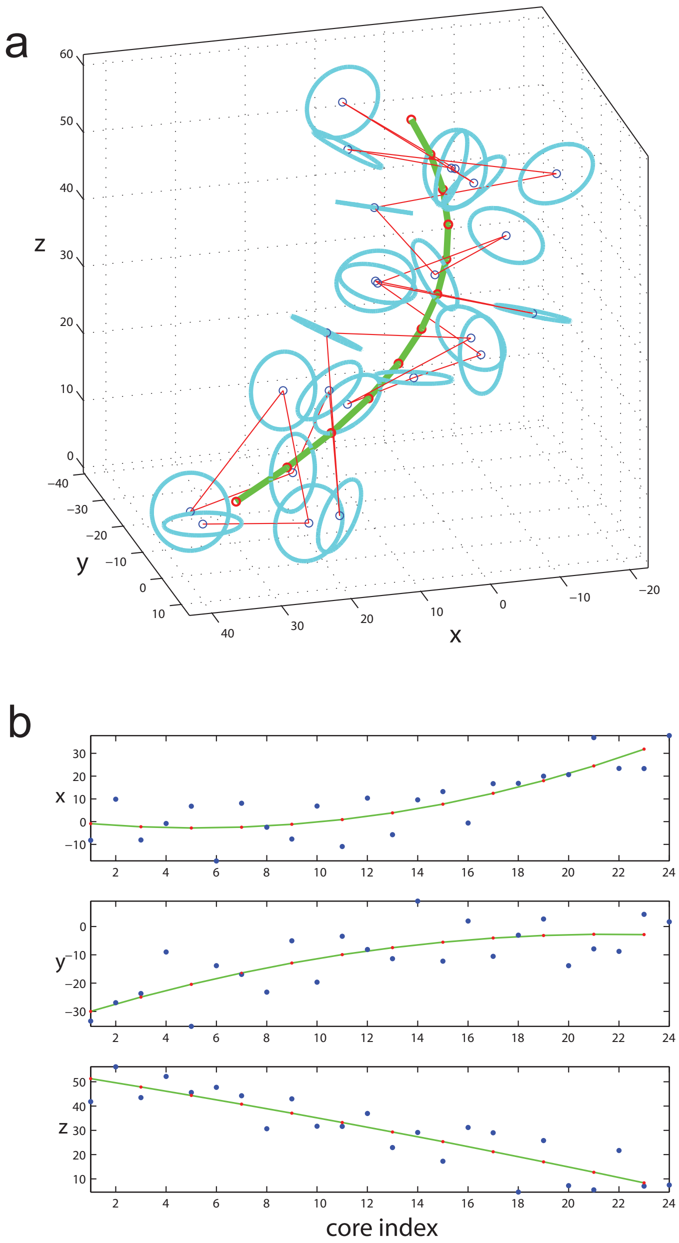
a
z
60
50
40
30
20
10
0
y
−40
−30
−20
−10
0
10
x
40
30
20
10
0
−10
−20
b
x
30
20
10
0
−10
y
0
−10
−20
−30
z
50
40
30
20
10
2
4
6
8
10
12
14
16
18
20
22
24
core index

Figure S5: