Modeling studies of chromatin fiber structure as a function of DNA linker length
Supplemental material

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q_l (e)	x	y	z (nm)	q_l (e)	x	y	z (nm)	q_l (e)	x	y	z (nm)	q_l (e)	x	y	z (nm)
-0.92	0.68	-0.17	1.94	0.28	-1.57	-4.04	1.71	-1.04	-4.14	2.60	-0.24	-0.45	1.34	-4.08	-1.56
-1.39	0.12	0.72	2.84	-1.98	-0.43	-4.73	1.77	-0.60	-4.38	1.15	-0.22	-1.30	3.64	-2.01	-1.48
-2.03	-0.50	-0.51	2.01	2.75	1.54	-2.64	1.08	-1.41	-4.84	-0.98	-0.24	-1.23	3.27	-1.25	-1.27
-2.53	1.23	0.81	2.16	-0.01	4.97	-1.26	1.87	-0.50	-4.88	-2.14	-0.25	-1.20	4.36	-0.27	-1.98
-0.06	-1.37	-0.74	2.86	-0.11	3.50	-0.95	1.30	-0.26	-2.25	-4.44	-0.22	-2.59	3.67	0.83	-1.74
2.31	0.33	-1.16	1.34	-2.40	4.97	0.31	1.45	-1.72	2.22	-3.52	-0.18	-2.01	3.58	3.02	-2.29
4.71	-1.11	0.62	2.37	-0.78	4.47	2.67	1.63	-2.04	3.42	-3.46	-0.20	-5.40	2.20	3.18	-1.96
-0.63	1.16	-0.27	0.86	3.14	3.22	3.03	1.37	-1.11	4.28	-1.94	-0.20	-0.20	0.34	3.22	-1.76
1.50	-0.51	1.96	2.90	-0.85	1.05	4.73	1.70	-0.76	4.31	2.42	-0.55	-2.47	-1.25	3.02	-1.85
-2.46	-1.41	-0.24	2.10	-0.93	-0.39	4.15	1.47	-0.98	3.24	3.47	-0.55	-3.24	-2.38	2.08	-1.83
-1.75	-0.80	-1.73	2.18	-1.28	-1.44	4.80	1.71	-2.11	-2.44	3.78	-0.57	-3.31	-3.07	1.23	-1.90
-0.76	1.34	2.38	2.88	-1.22	-3.20	3.95	1.76	-0.91	-4.70	1.95	-0.64	-1.29	-3.09	0.32	-1.78
-5.03	0.30	1.66	1.97	-1.46	-3.67	2.16	1.49	-2.29	-4.96	-0.14	-0.61	-1.35	-3.23	-1.56	-1.92
-0.03	-1.42	1.54	2.62	-1.79	-3.88	-1.48	1.44	-2.07	-4.13	-2.30	-0.50	1.41	-1.94	-2.79	-1.72
2.82	2.41	1.21	2.21	-1.49	-3.28	-3.54	1.54	-0.68	-3.31	-3.82	-0.59	-5.07	-1.24	-4.05	-2.05
-2.39	0.32	2.58	2.54	-1.69	-2.42	-3.94	1.45	-0.57	-0.51	-5.55	-0.61	-0.82	0.26	-4.10	-1.84
-0.65	-1.51	2.66	3.11	1.02	1.00	-3.90	1.14	-0.27	1.29	-5.72	-0.63	-0.38	0.73	-4.81	-2.26
0.31	-2.53	-0.42	2.59	-0.93	2.68	-3.79	1.31	-1.24	1.29	-2.96	-0.35	0.16	1.59	-5.07	-2.39
-0.74	0.03	-2.37	1.89	-1.47	3.03	-2.59	1.08	-0.67	2.94	-4.01	-0.52	-0.04	1.19	-2.48	-1.19
-1.70	2.30	0.14	1.47	1.52	2.27	-1.93	-0.76	-0.60	4.77	-1.41	-0.53	-0.29	2.87	0.01	-1.49
-1.84	2.07	2.14	2.26	-1.58	5.73	-0.76	-1.69	-0.85	5.10	0.99	-0.91	-0.40	4.11	1.30	-2.33
5.27	-0.88	2.66	2.46	-2.53	4.96	1.40	1.16	0.72	1.01	4.21	-0.85	1.25	2.76	1.33	-1.71
-0.84	-2.69	0.95	2.55	-1.99	4.02	3.32	1.27	-1.22	-1.48	4.43	-0.95	-0.43	1.95	3.89	-2.59
-0.65	-2.16	0.36	2.01	-1.94	2.16	4.68	1.26	-1.45	-3.68	3.54	-1.04	-0.46	-0.07	4.19	-2.61
-1.59	-2.49	-2.30	2.69	-0.66	0.25	4.83	1.23	0.23	-4.47	0.57	-0.90	-3.22	-0.96	3.81	-2.41
-1.55	1.06	-2.09	1.45	-2.24	-2.14	4.51	1.30	-1.08	-4.58	-1.58	-0.92	0.06	-2.13	3.05	-2.47
-0.45	4.12	0.53	2.52	-2.13	-3.67	3.33	1.31	-2.58	-3.57	-2.98	-0.83	1.55	-3.12	1.91	-2.38
0.12	3.81	1.78	2.64	-1.65	-4.57	0.80	1.22	-0.74	-1.57	-4.95	-0.94	-0.02	-3.77	1.61	-2.69
-1.84	1.80	2.98	2.38	-0.76	-3.99	-2.62	1.22	-1.49	0.45	-5.20	-0.69	-1.41	-2.14	-3.53	-2.36
-2.19	-2.54	2.14	2.52	-2.23	-1.88	-4.15	1.12	-0.33	1.31	-3.96	-0.67	-0.81	-1.01	-4.62	-2.58
-1.57	-1.69	1.29	1.71	-1.49	0.57	-5.12	1.23	-1.77	2.18	-2.63	-0.57	-2.26	-0.60	-3.22	-1.83
-0.82	-3.90	0.34	2.88	-0.39	1.47	-4.79	1.10	-0.61	4.17	-3.00	-0.87	1.29	0.32	-2.42	-1.23
-0.79	-3.61	-1.46	2.76	-0.23	2.31	-3.09	0.79	-2.32	4.95	0.05	-1.19	0.03	0.73	-3.47	-1.86
-1.71	-1.25	-3.29	2.26	-2.06	2.89	-1.17	0.61	-1.43	4.00	3.22	-1.30	1.36	0.69	-1.81	-0.94
-0.65	0.01	-3.48	2.12	-0.63	4.45	-1.15	1.06	-1.09	2.34	4.21	-1.27	-1.48	1.86	-1.12	-1.02
0.00	2.52	-1.03	1.46	-0.79	6.06	0.11	0.98	-1.96	-0.05	4.49	-1.25	-0.81	3.30	1.53	-2.29
-0.33	3.47	-0.05	1.73	-0.80	4.99	2.35	0.88	-2.26	-4.29	2.72	-1.44	-1.05	2.70	2.46	-2.47
-2.94	3.41	1.05	1.90	-2.96	2.78	3.89	0.80	-2.19	-4.84	1.32	-1.42	-2.84	1.25	2.73	-2.17
-1.83	3.00	1.90	1.97	-1.40	0.99	5.34	0.98	-0.73	-5.13	-0.80	-1.43	-1.11	0.84	3.51	-2.52
3.31	0.95	3.00	1.93	-0.81	-1.07	4.47	0.83	-0.66	-4.58	-2.45	-1.40	1.36	-0.21	2.40	-1.91
-3.12	-2.26	3.25	2.50	-0.78	-2.84	4.02	0.90	-3.75	-2.51	-4.22	-1.24	-0.04	-1.22	1.89	-1.88
-1.47	-3.53	1.84	2.53	0.82	-3.67	2.66	0.87	-0.69	-0.75	-4.98	-1.25	-2.30	-1.77	2.28	-2.32
-0.70	-3.21	0.22	2.13	-0.30	-4.38	-0.57	0.79	-0.74	0.22	-5.94	-1.46	1.14	-2.86	-0.42	-2.19
-2.66	-3.35	-0.82	2.17	-2.64	-2.88	-3.63	0.77	0.50	1.53	-4.84	-1.16	-0.56	-2.37	-2.05	-2.26
-3.31	-2.67	-1.59	1.92	-2.62	-0.99	-4.78	0.78	-3.39	3.20	-2.41	-0.93	0.64	-0.57	-2.34	-1.58
2.49	-1.74	-2.39	1.76	-2.08	2.01	-4.08	0.68	-0.76	4.39	-2.10	-1.14	-0.75	2.57	-1.26	-1.57
-1.18	-0.93	-4.17	2.31	-0.65	3.62	-3.37	0.78	-1.15	5.04	-0.87	-1.22	-0.66	1.90	1.57	-1.88
0.05	0.62	-3.00	1.52	0.16	5.47	-1.37	0.91	-3.52	4.37	1.73	-1.45	1.71	1.91	2.27	-2.37
-0.08	5.15	-1.27	2.75	-1.71	5.27	-0.41	0.88	-1.14	3.09	3.60	-1.51	0.78	0.47	2.59	-2.30
0.11	4.07	-1.05	2.12	0.05	5.24	0.62	0.47	-0.96	-0.86	4.44	-1.64	-0.31	-0.86	2.76	-2.63
-1.31	4.92	1.01	2.29	-2.07	4.09	2.67	0.50	-1.91	-2.71	3.12	-1.55	1.86	-2.86	0.89	-2.72
-2.56	4.17	1.42	1.97	-0.78	3.57	3.50	0.47	0.31	-4.08	1.84	-1.66	-0.53	-2.04	0.20	-1.99
-1.45	3.83	2.95	2.25	-3.13	1.91	4.20	0.45	-0.37	-3.80	0.00	-1.38	-0.20	-1.41	-2.89	-2.52
-0.85	1.54	4.13	-2.18	-1.78	-0.33	4.96	0.51	-1.74	-4.17	-0.89	-1.55	-1.51	2.54	0.57	-2.08
-0.34	-0.76	4.25	2.24	-2.54	-1.99	4.09	0.47	-2.75	-4.08	-1.76	-1.58	-4.17	1.27	2.08	-2.24
-3.39	-1.36	3.46	1.97	-1.23	-4.08	1.62	0.53	-0.85	-3.17	-3.51	-1.61	-0.72	-2.37	1.72	-3.07
1.50	-2.24	2.60	1.86	-1.22	-4.05	-1.85	0.44	-1.03	-1.94	-5.15	-1.80	-0.90	-2.60	-1.15	-2.77
-1.72	-4.00	1.02	2.19	-0.70	-0.07	-4.92	0.49	-4.17	0.07	-5.09	-1.61	3.12	-1.11	-2.22	-2.19
-0.71	-4.02	-2.19	2.29	-1.08	3.05	-4.17	0.44	-0.48	1.12	-5.52	-1.77	0.55	1.85	-0.22	-1.56
-1.38	-2.75	-3.71	2.22	-0.68	3.61	-1.97	0.33	2.85	1.38	-1.70	-0.61	-2.46	-0.27	1.29	-1.83
1.87	-2.03	-3.25	1.82	0.30	4.07	-1.34	0.39	4.63	2.58	-1.51	-0.86	2.57	-1.86	0.97	-2.73
-1.87	0.48	-4.36	1.93	-0.69	4.69	1.65	0.17	-1.56	3.82	-0.59	-1.17	-4.04	-1.44	-0.76	-2.01
-2.37	1.78	-3.26	1.55	0.92	2.49	3.89	0.11	-1.05	4.84	0.83	-1.90	-2.25	-1.61	-1.50	-2.48
2.83	1.85	-0.94	0.78	-1.36	0.65	4.79	0.13	2.45	3.17	2.26	-1.57	0.65	0.54	1.79	-2.54
-0.72	4.97	-0.33	2.18	0.89	-1.33	4.31	0.19	-3.06	1.41	3.86	-1.78	2.44	-0.97	1.12	-2.40
-1.16	5.90	0.03	2.18	-0.89	-3.21	3.31	0.16	-1.21	0.54	4.50	-1.99	-1.97	-0.59	-1.43	-1.79
-0.75	4.96	2.10	2.03	-0.14	-4.88	0.33	0.13	-2.01	-1.95	4.01	-2.03	-2.01	1.33	0.64	-1.87
-1.26	2.76	3.86	1.88	2.43	-3.55	-2.91	0.17	-2.62	-3.46	2.58	-1.99	0.16	-1.76	0.17	-3.02
-0.58	0.61	3.92	1.65	-2.40	0.96	-4.90	0.16	-2.56	-4.03	0.85	-1.90	-0.30	0.29	-1.58	-1.71
-2.27	-0.24	3.33	1.71	-1.33	1.70	-4.58	0.11	0.62	-3.43	-0.68	-1.61	-0.55	0.95	-0.95	-1.12
0.10	-2.14	4.11	2.06	-1.56	4.21	-2.78	0.15	-0.09	-4.07	-2.63	-1.98	-2.71	-1.10	0.03	-2.36
0.81	-3.26	2.86	1.90	-2.75	4.97	-0.98	0.11	-3.11	-3.11	-2.51	-1.73	-4.99	0.41	0.69	-1.90
-1.18	-4.24	1.77	2.06	-1.02	4.98	-0.07	-0.17	-0.67	-2.80	-4.17	-2.08	-5.50	-0.53	-0.45	-1.82
-1.56	-4.56	-0.22	1.95	-0.86	1.63	4.95	-0.19	-0.96	0.48	-5.85	-2.25	1.26	-0.35	0.43	-2.82
-4.07	-3.16	-2.72	1.75	-0.86	-0.58	4.54	-0.22	-0.95	0.32	-3.26	-1.25	4.14	0.77	-0.12	-1.57

Table S1: Nucleosome pseudo-charges and relative postions on the nucleosome surface at $C_S = 0.15$ M obtained with the DiSCO approach.

Parameter	Description	Value
T	Temperature	293.15° K
C_S	Monovalent salt concentration (NaCl)	0.15 M
l_0	Equilibrium DNA segment length	3.0 nm
L_p	Persistence length of linker DNA in monovalent salt	50 nm
h	Stretching rigidity of linker DNA	$100 k_B \mathrm{T}/l_o^2$
g	Bending rigidity of linker DNA	$L_p k_B \mathrm{T}/l_o$
s	Torsional rigidity constant of linker DNA	3.0×10^{-12} erg.nm
θ_0	Angular separation between linker segments at core	108°
$2w_0$	Width of wound DNA supercoil	3.6 nm
r_0	Radius of wound DNA supercoil	4.8 nm
σ_{tt}	Excluded vol. distance for tail/tail interactions	1.8 nm
σ_{tc}	Excluded vol. distance for tail/core interactions	1.8 nm
σ_{cc}	Excluded vol. distance for core/core interactions	1.2 nm
σ_{tl}	Excluded volume distance for tail/linker DNA interactions	2.7 nm
σ_{cl}	Excluded vol. distance for core/linker DNA interactions	2.4 nm
σ_{gLHc}	Excluded vol. distance for globular link. hist./core interactions	2.2 nm
σ_{gLH1}	Excluded vol. distance for globular link. hist./link.DNA interactions	3.4 nm
σ_{cLHc}	Excluded vol. distance for C-term. link. hist./core interactions	2.4 nm
σ_{cLH1}	Excluded vol. distance for C-term. link. hist./link.DNA interactions	3.6 nm
k_{ev}	Excluded vol. energy param for all components except for tail beads	0.001 $k_B T$
k_{evt}	Tail/tail excluded volume interaction energy parameter	0.1 $k_B T$
q_{gLH}	Charge on the globular linker histone bead	13.88e
q_{cLH}	Charge on the C-terminal linker histone bead	25.62e
σ_{LHLH}	Excluded volume distance for link.histone/link.histone interactions	2.0 nm

Table S2: Parameters employed in mesoscale modeling/simulation.

Tail	Bond i-j	k_b (kcal/mol/ÅÅ)	Average [Å]	SD [Å]
N-ter H3	1-2	0.09	15.6	2.3
	2-3	0.06	15.0	3.0
	3-4	0.07	15.6	2.9
	4-5	0.07	16.1	2.6
	5-6	0.07	16.1	2.6
	6-7	0.07	15.1	2.9
	7-8	0.11	14.9	2.4
N-ter H4	1-2	0.10	14.1	2.6
	2-3	0.10	15.2	2.4
	3-4	0.06	14.8	2.8
	4-5	0.20	14.7	1.8
N-ter H2A	1-2	0.08	14.1	2.6
	2-3	0.09	15.3	2.5
	3-4	0.03	14.5	3.4
C-ter H2A	1-2	0.07	15.7	2.6
	2-3	0.07	13.7	2.6
N-ter H2B	1-2	0.08	14.7	3.1
	2-3	0.10	14.1	2.3
	3-4	0.08	16.2	2.4
	4-5	0.08	15.1	2.7

Table S3: Protein bead stretching parameters.

Tail	Angle i-j	k_θ (kcal/mol/ÅÅ)	Average [Å]	SD [Å]
N-ter H3	1-2-3	1.1	108.6	28.8
	2-3-4	1.0	108.1	28.6
	3-4-5	1.7	111.3	25.4
	4-5-6	1.2	117.6	27.8
	5-6-7	1.2	110.4	29.3
	6-7-8	1.5	110.5	27.2
N-ter H4	1-2-3	1.0	103.2	25.4
	2-3-4	1.1	106.0	25.8
	3-4-5	0.5	103.6	35.5
N-ter H2A	1-2-3	1.1	108.5	29.0
	2-3-4	0.6	100.1	29.3
C-ter H2A	1-2-3	1.0	100.7	31.8
N-ter H2B	1-2-3	0.9	104.9	35.1
	2-3-4	0.6	103.9	28.4
	3-4-5	1.6	113.8	26.7

Table S4: Protein bond-angle parameters.
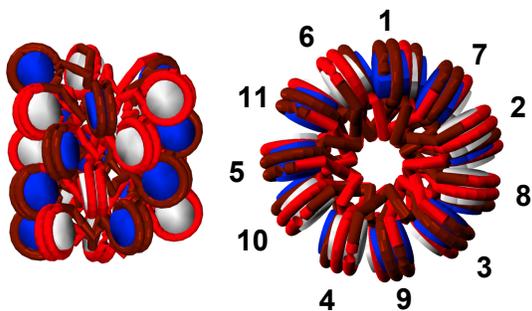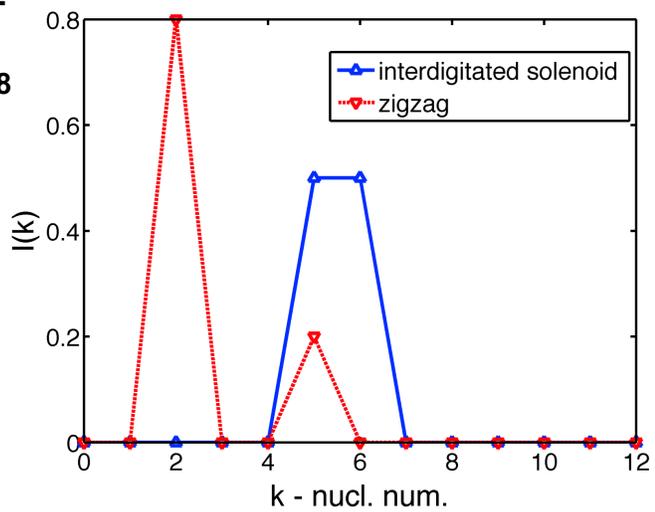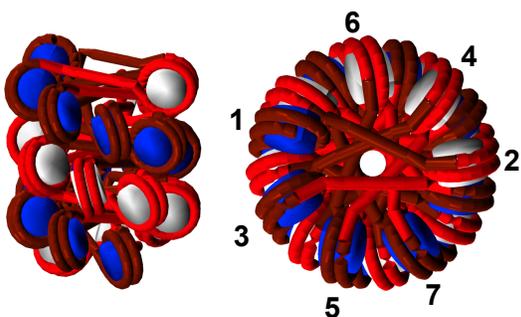
Figure S1: Initial configurations and their interaction patterns.
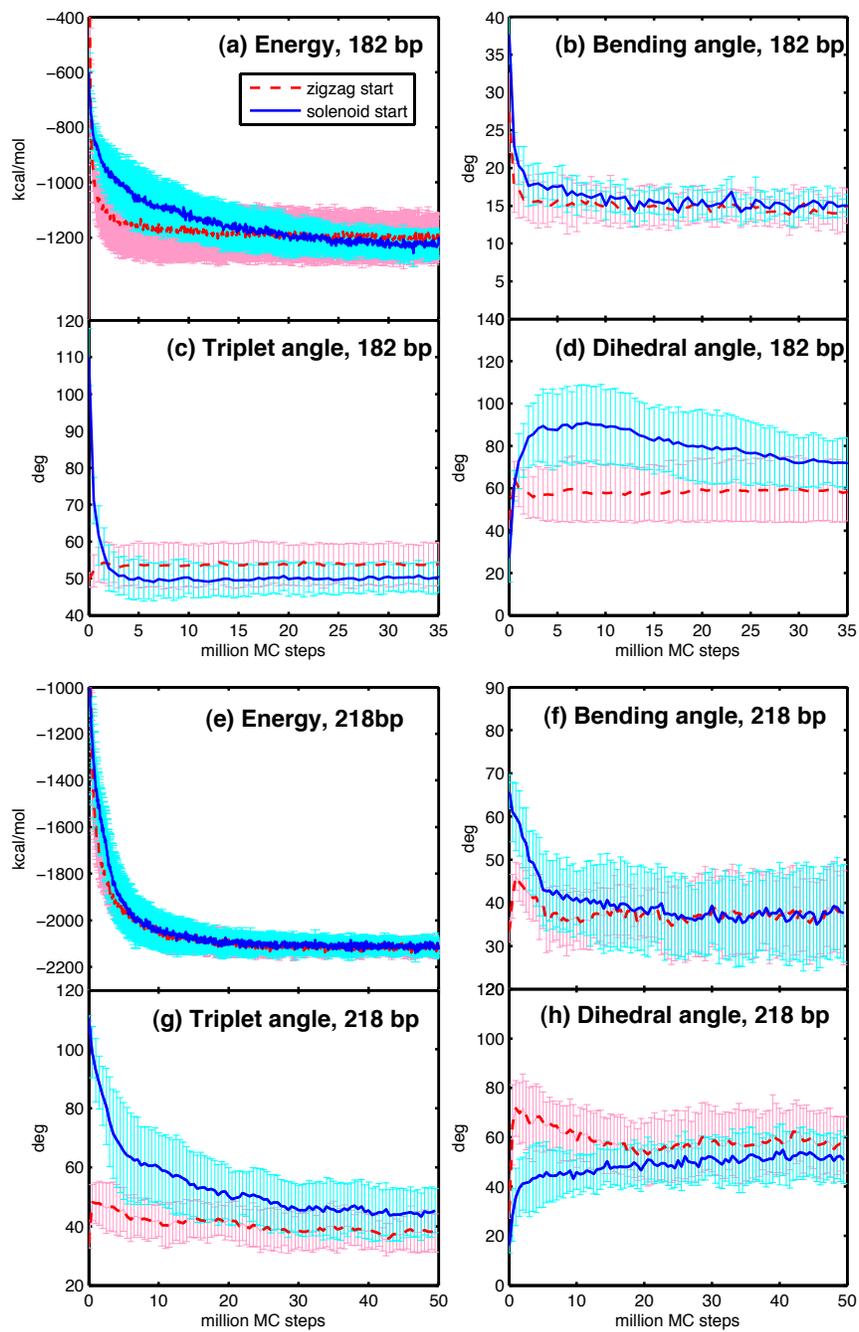
Figure S2: Convergence of different quantities for 24-core 182-bp (top half) and 218-bp (bottom half) oligonucleosome trajectories simulated with LH.

6
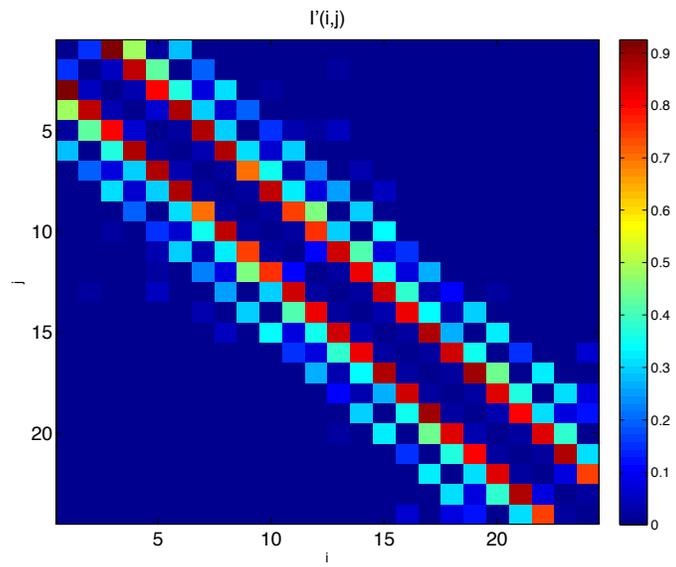
Figure S3: Internucleosome interaction matrix $I'(i, j)$.
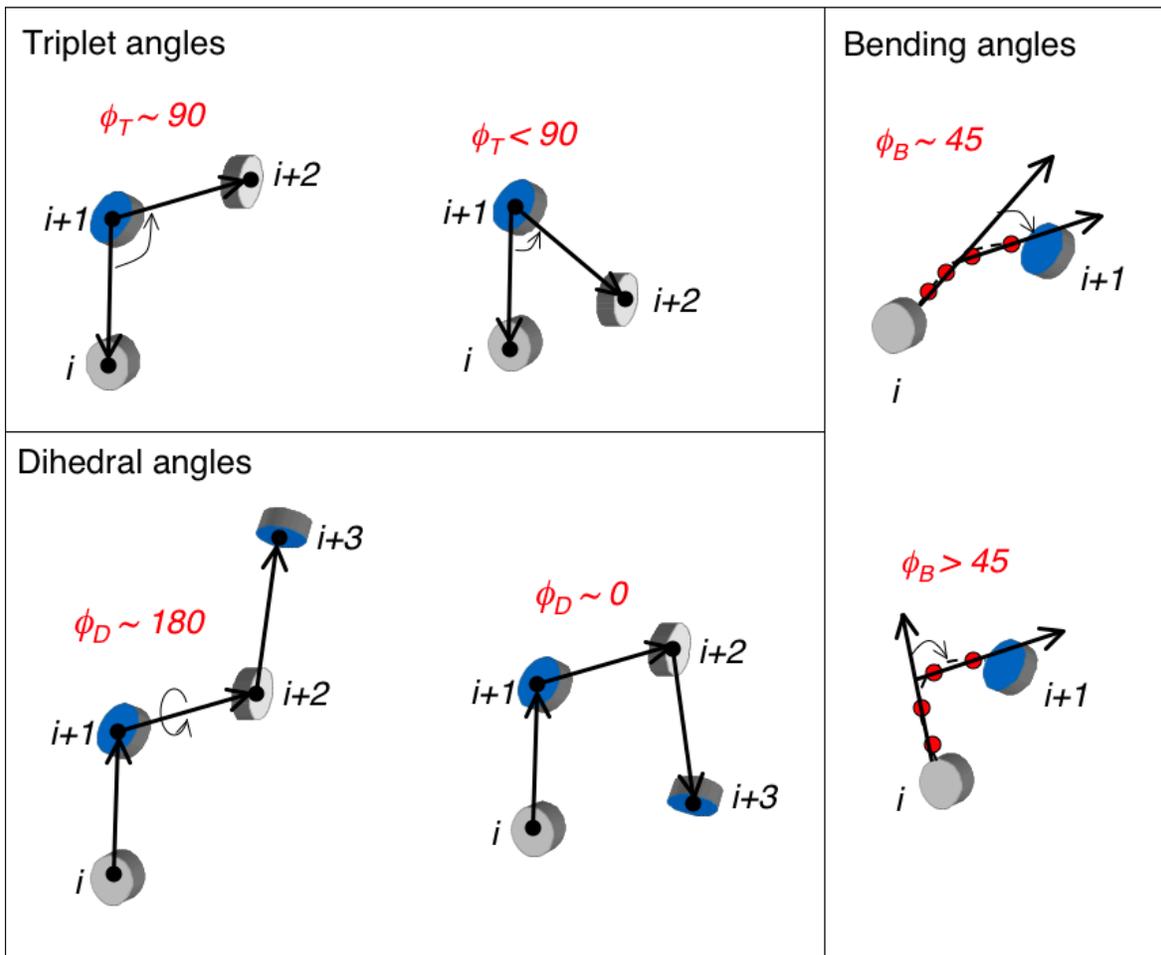
Figure S4: Triplet, dihedral, and bending angles cartoons.
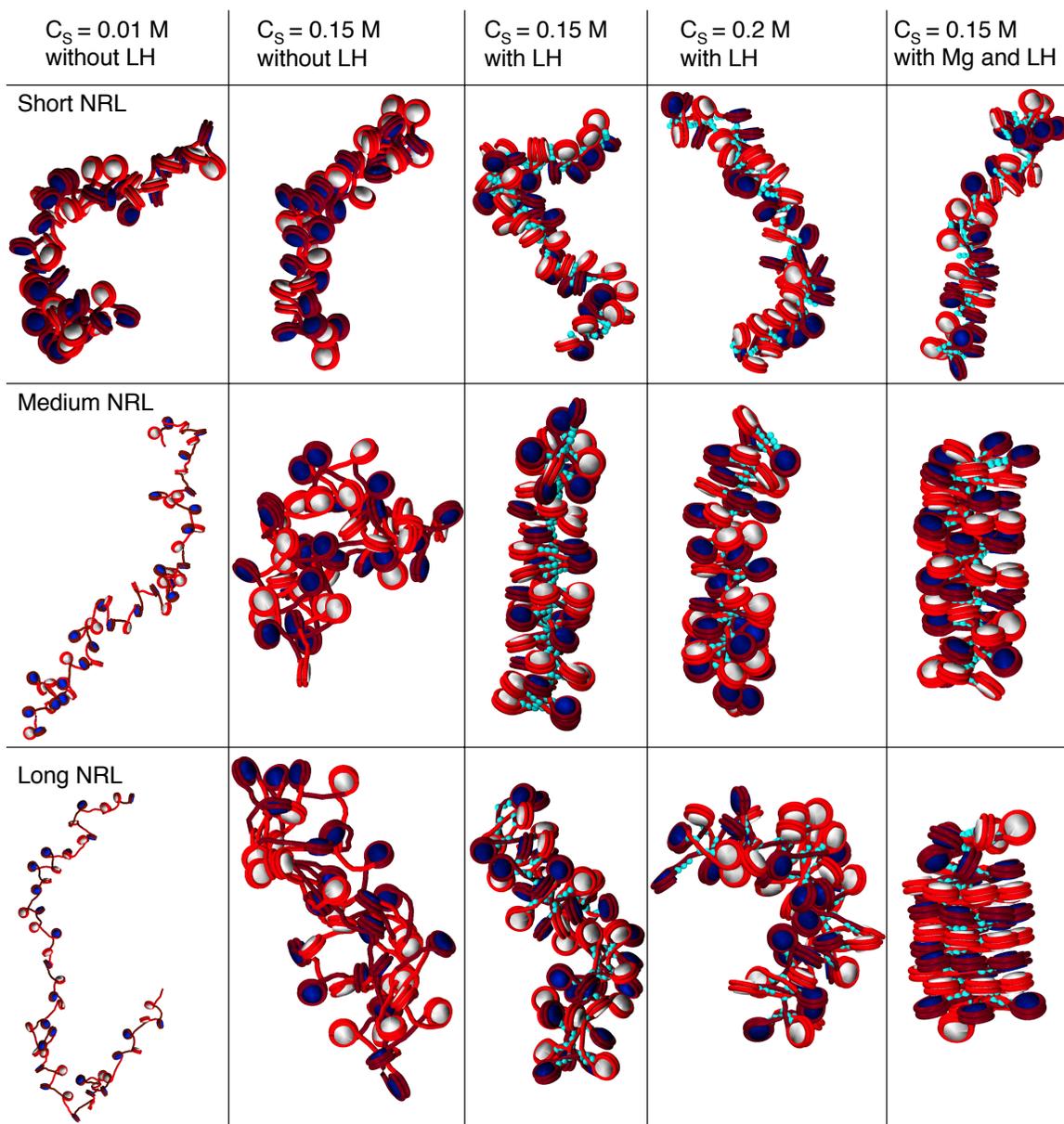
Figure S5: Space filling model for representative 48-core arrays (short NRL: 173 bp, medium NRL: 209 bp, and long NRL: 226 bp) at different salt concentrations. Nucleosomes, DNA linkers, and LH are colored as in Figure 2.
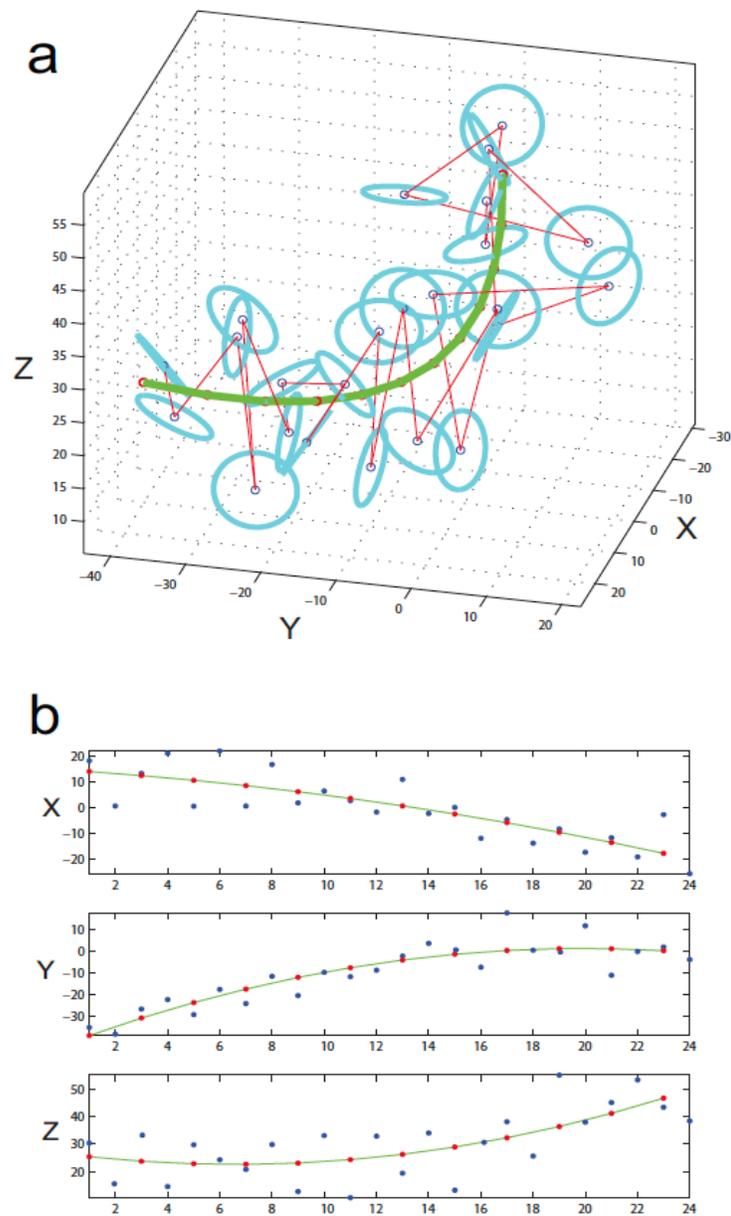
Figure S6: Description of the fiber axis calculation for 24-unit oligonucleosome. (a) Cyan - nucleosome cores, Red lines - connections between consecutive nucleosomes, Green line - fiber axis, as estimated by the least squares procedure; (b) Fiber axis decomposition into three separate curves for three vectors (x, y, and z); Blue dots - nucleosome centers, Green line - fiber axis, Red dots - separators between line segments of the fiber axis.
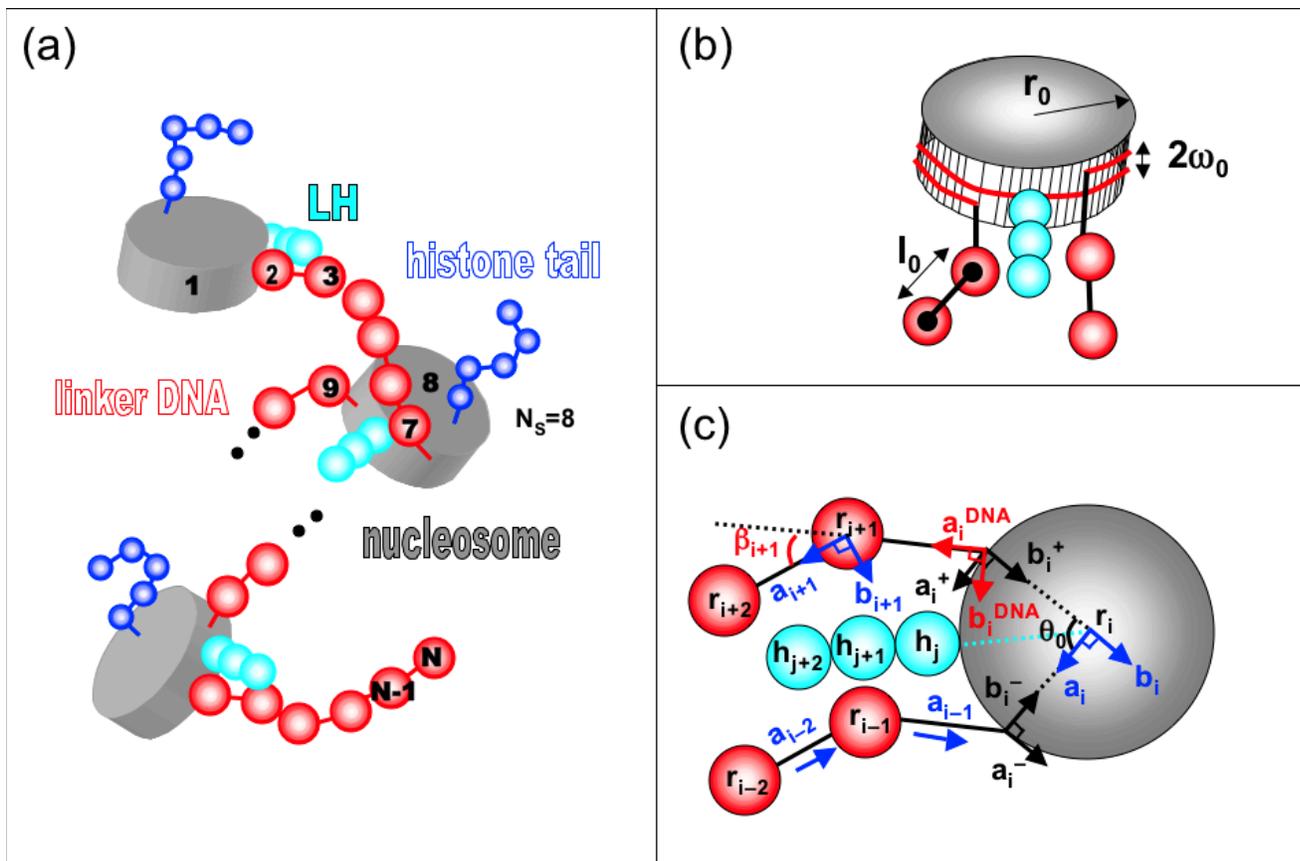
Figure S7: Geometry of the mesoscale oligonucleosome showing (a) assembly of oligonucleosome components into a chain, (b) entering/exiting linker DNA, and (c) individual coordinate systems for the linker DNA beads and nucleosome core, and Euler angle β depicting the linker DNA bending. For nucleosome core i, $\mathbf{a}_i$ and $\mathbf{b}_i$ lie in the nucleosome core plane, with $\mathbf{a}_i$ pointing along the tangent at the attachment site of the entering DNA, and $\mathbf{b}_i$ in the direction normal to this tangent. For linker DNA bead i, the vector $\mathbf{a}_i$ points from the geometric center of i to either the center of the following DNA bead or to the attachment point in the nucleosome (if $i+1$ is a core). The vector $\mathbf{a}_i^{\mathrm{DNA}}$ points from the attachment point of the exiting linker DNA to the center of the following DNA linker bead. The vectors $\mathbf{a}_i^+$ and $\mathbf{a}_i^-$ represent the local tangents on the nucleosome cores at the exiting and entering points of attachment, respectively.