Recovering Ensembles of Chromatin Conformations from Contact Probabilities – Supplementary Data
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Table S1. Harmonic restraints used when simulating test systems and when performing the ensemble recovery procedure.

N [b]	Loops [c]		n^* [d]	i,j [e]	$k_{i,j}$ [f]	n [g]	i,j [h]	$k_{i,j}(2)$ [i]	$k_{i,j}(n+1)$ [j]
25	2	free	3	13, 23	2.5	3	13, 23	2.462	2.506
				3, 13	2.5		3, 13	2.552	2.544
				3, 23	2.5		3, 23	2.558	2.544
25	2	tied	4	13, 23	2.5	4	13, 23	2.564	2.518
				3, 13	2.5		3, 13	2.558	2.591
				3, 23	2.5		3, 23	2.406	2.521
				8, 18	2.5		8, 18	2.489	2.411
35	3	free	4	13, 23	2.5	6	13, 23	2.539	2.634
				23, 33	2.5		23, 33	2.509	2.485
				3, 13	2.5		3, 13	2.512	2.494
				3, 33	2.5		3, 33	2.500	2.531
							13, 33	0.000	0.000
							3, 23	0.000	0.000
35	3	tied	6	13, 23	2.5	9	13, 23	2.539	2.645
				18, 28	2.5		18, 28	2.610	2.706
				23, 33	2.5		23, 33	2.387	2.284
				3, 13	2.5		3, 13	2.413	2.446
				3, 33	2.5		3, 33	2.505	2.597
				8, 18	2.5		8, 18	2.665	2.607
							11, 27	0.000	0.000
							13, 33	0.000	0.000
							3, 23	0.162	0.019
45	4	free	5	13, 23	2.5	10	13, 23	2.520	2.456
				23, 33	2.5		23, 33	2.549	2.501
				3, 13	2.5		3, 13	2.463	2.496
				3, 43	2.5		3, 43	2.524	2.527
				33, 43	2.5		33, 43	2.521	2.546
							13, 33	0.000	0.000
							13, 43	0.000	0.000
							23, 43	0.002	0.000
							3, 23	0.000	0.000
							3, 33	0.000	0.000
45	4	tied	8	13, 23	2.5	13	13, 23	2.297	2.367
				18, 28	2.5		18, 28	2.555	2.654
				23, 33	2.5		23, 33	2.305	2.664
				28, 38	2.5		28, 38	2.670	2.516
				3, 13	2.5		3, 13	2.411	2.402
				3, 43	2.5		3, 43	2.385	2.480
				33, 43	2.5		33, 43	2.190	2.255
				8, 18	2.5		8, 18	2.484	2.591
							13, 43	0.317	0.081
							14, 32	0.089	0.000
							24, 42	0.243	0.328
							3, 23	0.000	0.141
							4, 32	0.000	0.000

[a] Each test system is shown schematically as a straight chain of black beads with additional harmonic restraints represented by gray arcs connecting the restrained beads.   [b] Number of beads in the chain.   [c] Number and type of induced loops. Free loops result from connecting loop end-beads with harmonic restraints, shown as gray arcs in the schematics, while tied loops result from connecting middle beads across free loops, shown as dotted gray arcs in the schematics.   [d] Number of harmonic restraints used to induce the loops in the test system.
[e] Indexes of beads connected by harmonic restraints in the test systems. The first bead has index 1.   [f] Spring constant used for harmonic restraints in simulations of test systems.   [g] Number of harmonic restraints used during the ensemble recovery procedure.   [h] Indexes of beads connected by harmonic restraints during the ensemble recovery procedure.   [i] Restraint spring constants recovered for optimal conformation ensemble when using two parameters in the general linear model to predict spring constants from contact probabilities (CPs).
[j] Same as $k_{i,j}(2)$, but using $n+1$ parameters in the general linear model.