

SUPPORTING INFORMATION

Analyzing Ion distributions around DNA: sequence-dependence of potassium ion distributions from microsecond molecular dynamics

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SUPPORTING FIGURES

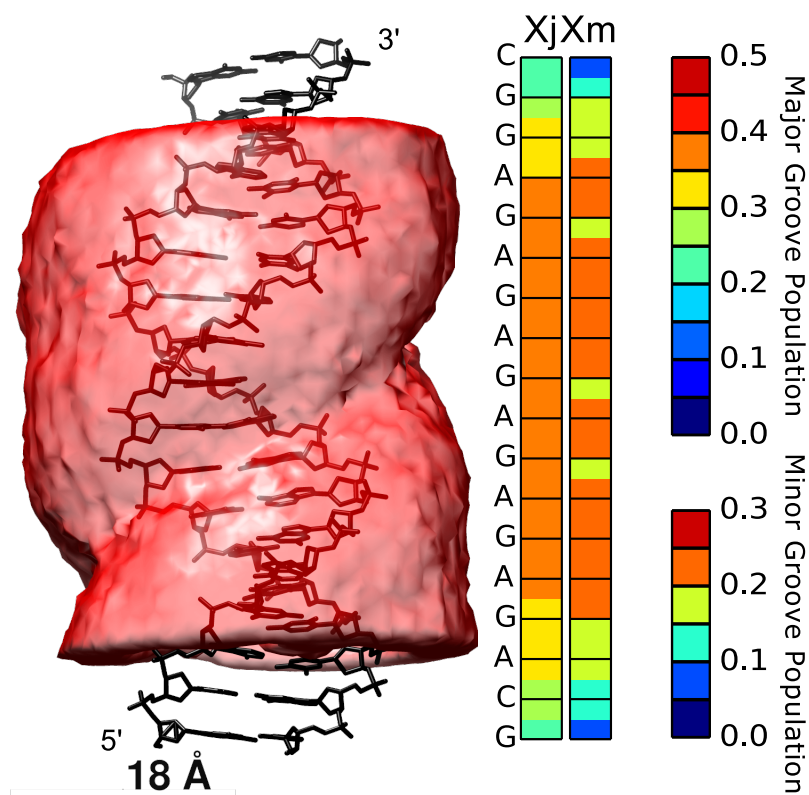


Figure S1: K⁺ molarity and population along the helix. Two representations of the K⁺ atmosphere in the outer (X) region surrounding the AGAG oligomer are presented. Left: Cartesian K⁺ isodensity surface at 0.6 M (red, see caption to figure 4); the average structure is shown in stick representation to highlight the position of the major and minor grooves; the 5' and 3' ends of the Watson strand are marked. The black horizontal line indicates a distance of 18 Å from the helical axis. Right: K⁺ population along the oligomer (5'-3' direction upwards) in the external region of the major (X_j) and minor (X_m) grooves, using the color schemes shown by the right-hand bars: populations increase from blue to red in increments of 0.05. Each base pair step is split into two half steps. See figure 1 for a precise definition of the grooves, and of the external groove region.

Figure S2

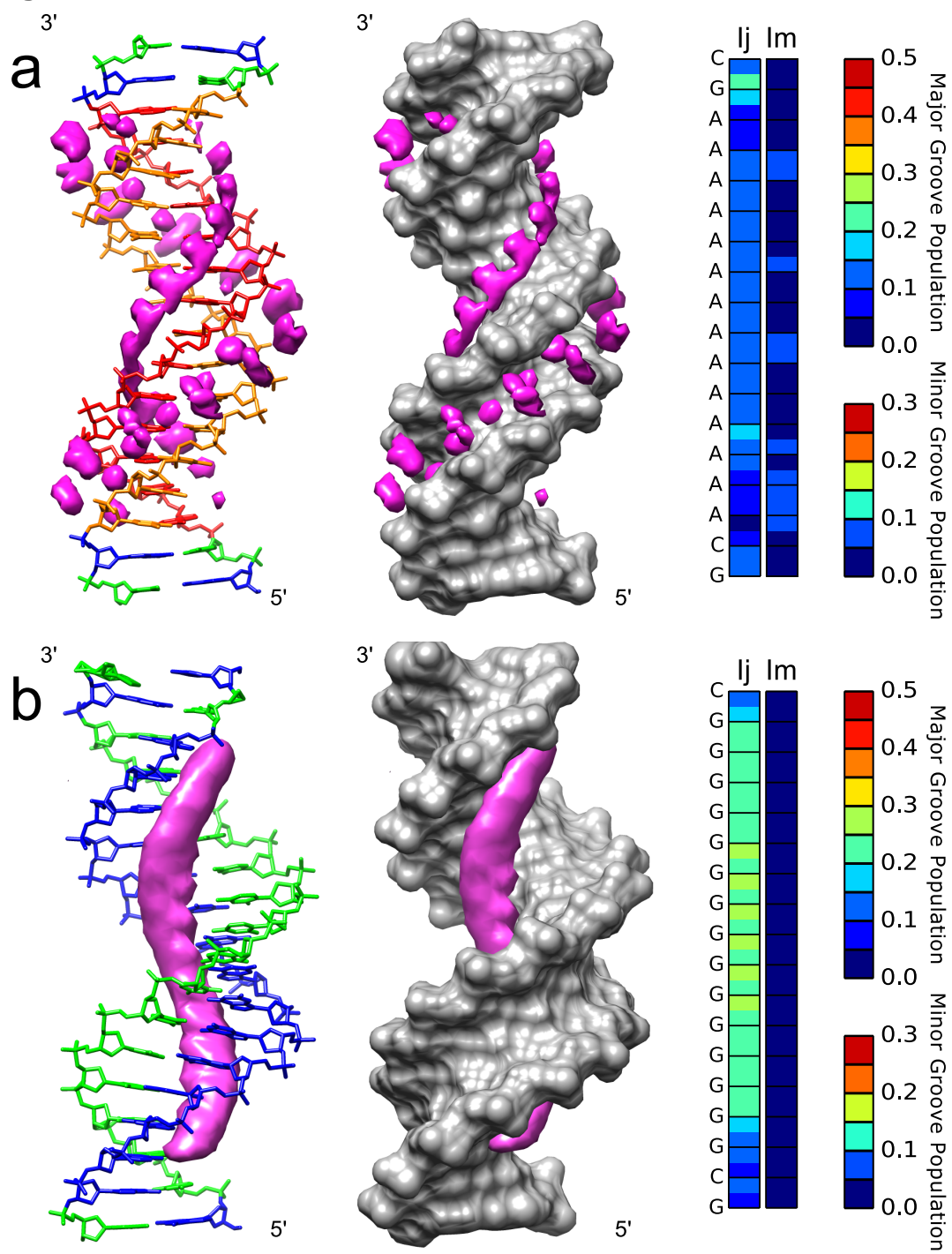


Figure S2 (...cont)

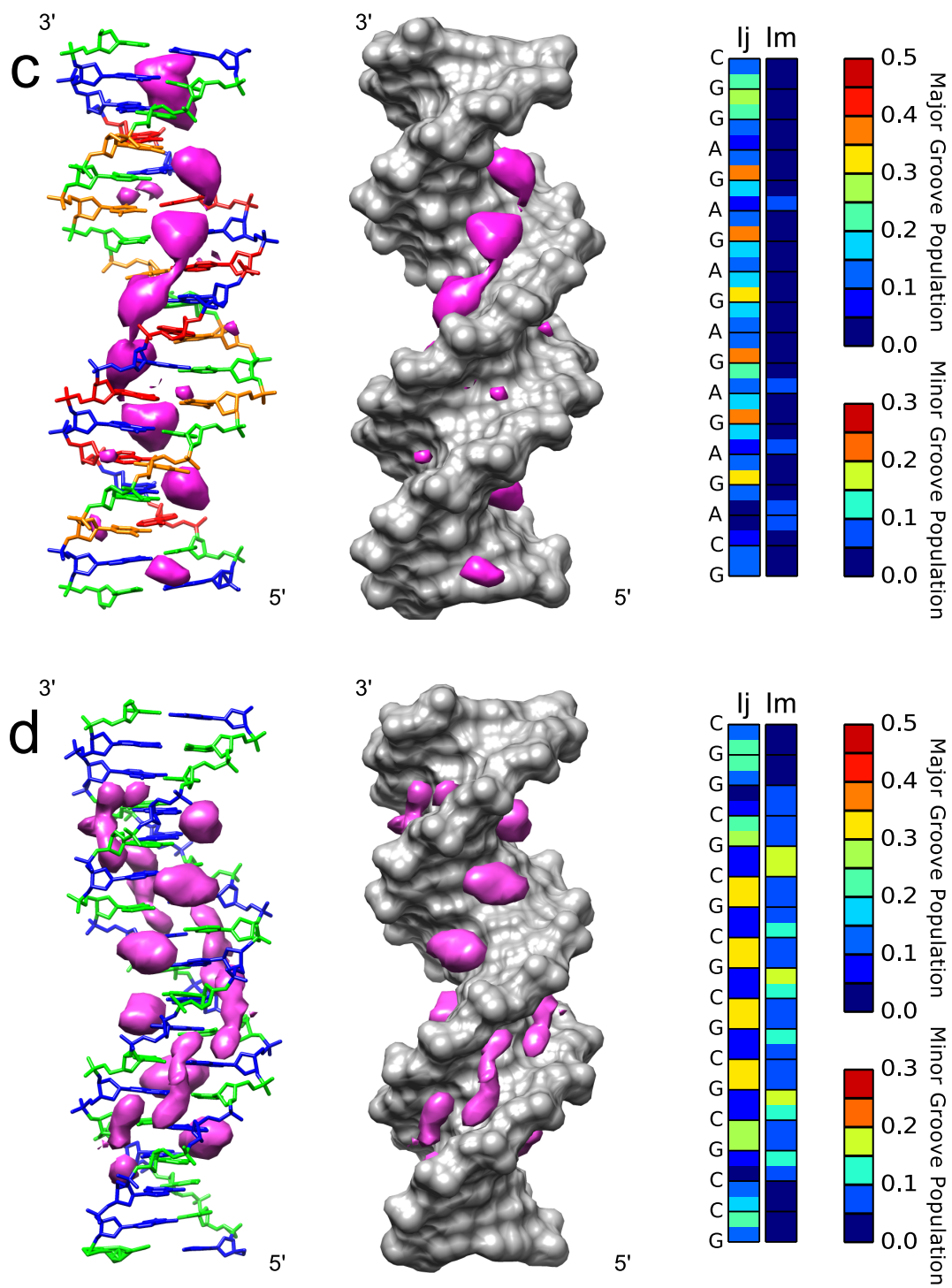


Figure S2 (...cont)

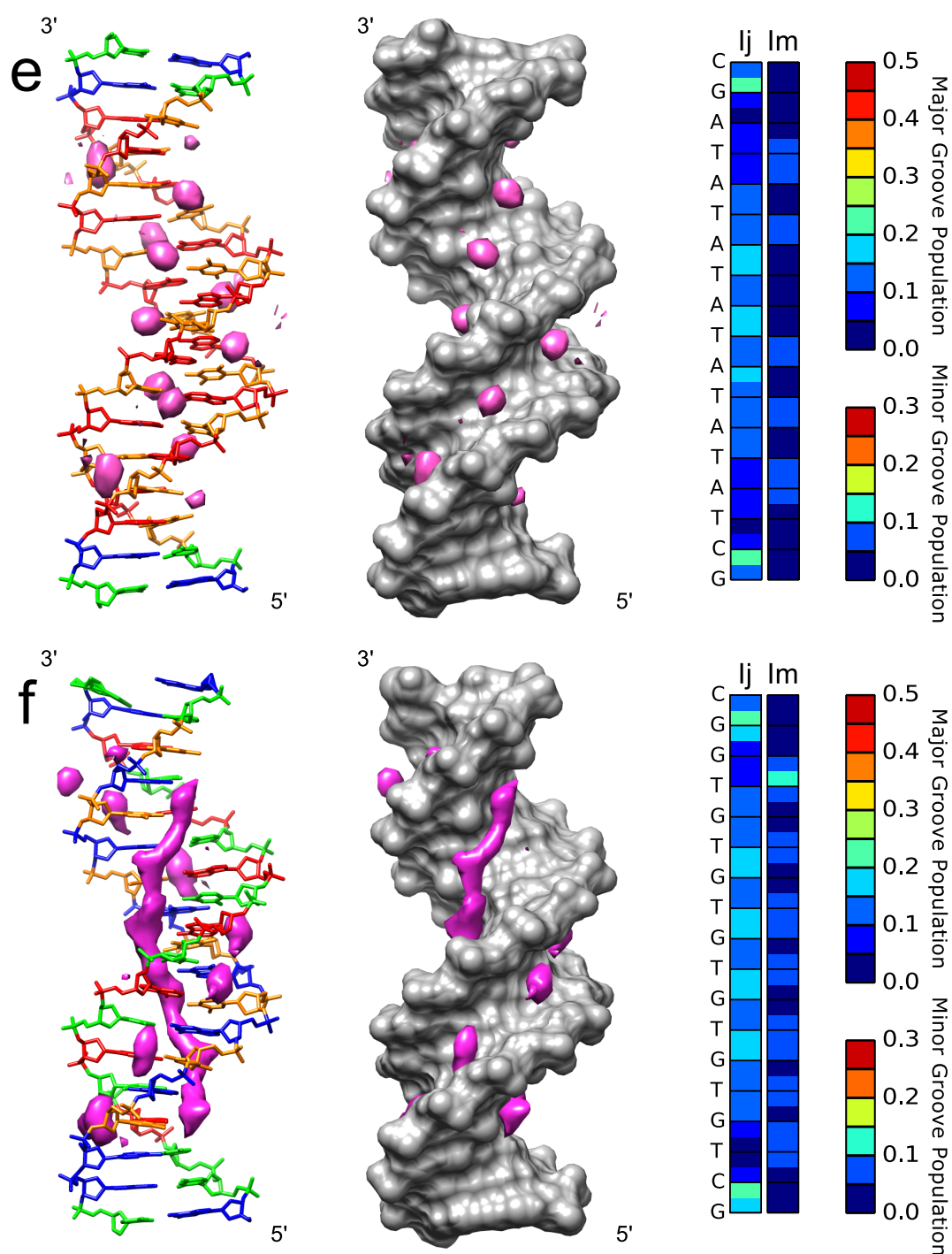


Figure S2: K⁺ density and population along 6 oligomers. The K⁺ atmosphere around the AAAA (a), GGGG (b), AGAG (c), CGCG (d), TGTG (e) and TATA (f) oligomers. (a-f) left and center: The cartesian K⁺ isodensity surface at 3 M (purple) is superposed on the corresponding average DNA structure, represented with colored sticks (left, see caption to figure 4), or its surface (center); the 5' and 3' ends of the Watson strand are marked. (a-f), right: K⁺ population along the oligomer (5'-3' direction upwards) inside the major (Ij) and minor (Im) grooves, using the displayed color scheme: population increases from blue to red in steps of 0.05. Each base pair step is split into two half steps; see figure 1 for a precise definition of the grooves.

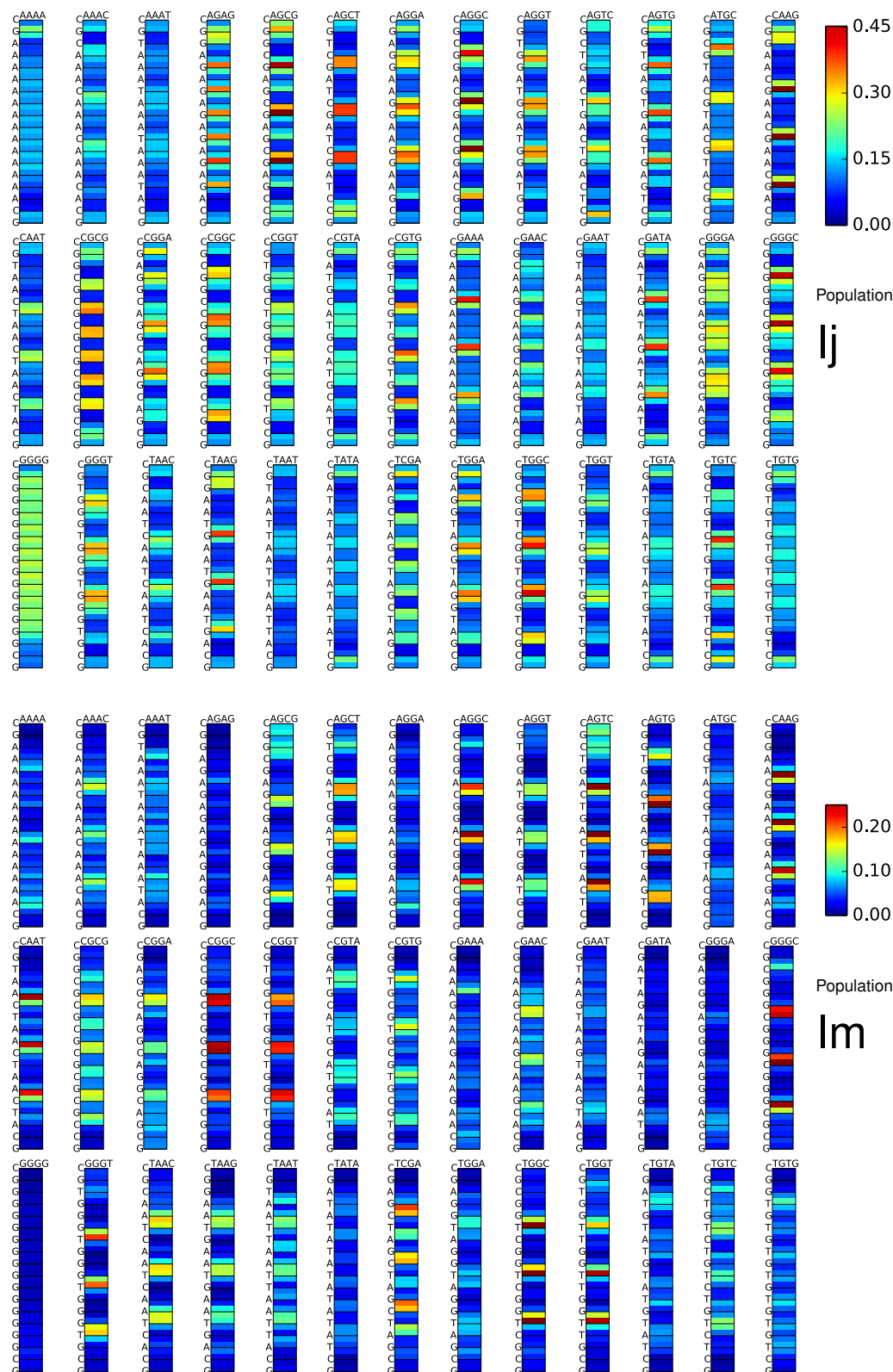


Figure S3: K⁺ population along the 39 oligomers. The K⁺ population along the full-length of the entire set of 39 oligomers within the major (Ij, top) and minor (Im, bottom) grooves, represented using the displayed color scheme, where population increases continuously from blue to red. The 5'-3' direction points upwards. Each base pair step is split into two half steps; see figure 1 for a precise definition of the grooves. The 39 oligomers are listed in alphabetical order.

Figure S4

Ij

Steps											Levels	
T..T	0.41	0.49	0.25	0.23	0.84	0.39	0.29	0.24	0.20	0.17	0.27	0.28
T..C	0.32	0.49	0.20	0.24	0.71	0.28	0.27	0.19	0.15	0.14	0.32	0.36
C..T	0.40	0.45	0.21	0.20	0.83	0.40	0.28	0.23	0.15	0.14	0.23	0.27
C..C	0.36	0.51	0.21	0.24	0.70	0.32	0.24	0.18	0.15	0.15	0.28	0.39
C..G	0.31	0.35	0.18	0.15	0.65	0.37	0.23	0.14	0.14	0.12	0.14	0.23
T..G	0.29	0.30	0.19	0.16	0.63	0.34	0.23	0.15	0.15	0.14	0.15	0.20
T..A	0.41	0.35	0.24	0.20	0.57	0.31	0.21	0.15	0.15	0.13	0.17	0.28
C..A	0.45	0.38	0.27	0.22	0.63	0.36	0.23	0.15	0.13	0.14	0.16	0.31
A..C	0.45	0.62	0.20	0.25	0.74	0.40	0.24	0.36	0.24	0.15	0.31	0.59
A..T	0.55	0.61	0.27	0.26	0.77	0.42	0.29	0.30	0.23	0.16	0.27	0.48
G..T	0.54	0.52	0.26	0.26	0.74	0.40	0.24	0.36	0.27	0.15	0.34	0.56
G..C	0.46	0.53	0.24	0.24	0.70	0.37	0.24	0.39	0.22	0.14	0.41	0.66
A..A	0.67	0.53	0.34	0.26	0.84	0.58	0.29	0.24	0.22	0.17	0.23	0.58
A..G	0.52	0.50	0.24	0.20	0.83	0.57	0.28	0.23	0.17	0.14	0.17	0.36
G..A	0.55	0.41	0.30	0.22	0.71	0.49	0.27	0.19	0.17	0.14	0.26	0.62
G..G	0.49	0.38	0.23	0.19	0.70	0.50	0.24	0.18	0.18	0.15	0.23	0.43
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G
max	0.67	0.62	0.34	0.26	0.84	0.58	0.29	0.39	0.27	0.17	0.41	0.66
mean	0.45	0.46	0.24	0.22	0.72	0.41	0.25	0.23	0.18	0.15	0.25	0.41
min	0.29	0.30	0.18	0.15	0.57	0.28	0.21	0.14	0.13	0.12	0.14	0.20
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G

Im

Steps											Levels	
T..T	0.05	0.10	0.08	0.11	0.08	0.09	0.12	0.14	0.20	0.26	0.10	0.09
T..C	0.06	0.09	0.10	0.12	0.06	0.13	0.09	0.28	0.42	0.27	0.18	0.16
C..T	0.07	0.09	0.08	0.10	0.05	0.11	0.10	0.07	0.16	0.24	0.12	0.12
C..C	0.06	0.10	0.09	0.11	0.07	0.13	0.15	0.27	0.42	0.46	0.25	0.19
C..G	0.06	0.09	0.09	0.12	0.12	0.16	0.12	0.34	0.44	0.48	0.31	0.26
T..G	0.05	0.11	0.09	0.13	0.08	0.13	0.13	0.33	0.36	0.44	0.21	0.16
T..A	0.06	0.09	0.07	0.11	0.07	0.11	0.09	0.24	0.36	0.34	0.21	0.19
C..A	0.08	0.12	0.17	0.13	0.08	0.12	0.13	0.33	0.49	0.44	0.30	0.23
A..C	0.02	0.06	0.07	0.08	0.04	0.06	0.11	0.10	0.10	0.11	0.08	0.03
A..T	0.01	0.03	0.03	0.12	0.04	0.06	0.17	0.05	0.05	0.06	0.09	0.03
G..T	0.01	0.06	0.04	0.08	0.04	0.07	0.11	0.10	0.10	0.11	0.10	0.03
G..C	0.03	0.06	0.05	0.13	0.05	0.06	0.17	0.16	0.26	0.29	0.10	0.03
A..A	0.05	0.07	0.08	0.04	0.08	0.09	0.12	0.14	0.13	0.26	0.10	0.06
A..G	0.03	0.05	0.07	0.10	0.05	0.07	0.10	0.07	0.14	0.24	0.09	0.03
G..A	0.05	0.08	0.07	0.11	0.06	0.11	0.09	0.28	0.46	0.27	0.12	0.05
G..G	0.03	0.08	0.07	0.12	0.07	0.07	0.15	0.27	0.33	0.46	0.08	0.03
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G
max	0.08	0.12	0.17	0.13	0.12	0.16	0.17	0.34	0.49	0.48	0.31	0.26
mean	0.05	0.08	0.08	0.11	0.06	0.10	0.12	0.20	0.28	0.30	0.15	0.11
min	0.01	0.03	0.03	0.04	0.04	0.06	0.09	0.05	0.05	0.06	0.08	0.03
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G

Figure S4, (...cont)

X_j

Steps											Levels	
T..T	0.81	0.80	0.81	0.80	0.77	0.77	0.76	0.82	0.81	0.76	0.81	0.80
T..C	0.77	0.78	0.77	0.78	0.73	0.73	0.76	0.74	0.70	0.75	0.77	0.75
C..T	0.80	0.78	0.79	0.81	0.76	0.76	0.75	0.84	0.79	0.76	0.80	0.78
C..C	0.78	0.78	0.76	0.80	0.72	0.72	0.73	0.74	0.70	0.68	0.76	0.74
C..G	0.78	0.79	0.77	0.77	0.75	0.76	0.77	0.74	0.70	0.68	0.77	0.76
T..G	0.78	0.78	0.77	0.78	0.76	0.80	0.77	0.76	0.75	0.71	0.79	0.79
T..A	0.82	0.83	0.84	0.80	0.78	0.80	0.80	0.82	0.78	0.73	0.80	0.79
C..A	0.78	0.79	0.78	0.81	0.76	0.77	0.77	0.76	0.72	0.71	0.79	0.77
A..C	0.72	0.75	0.71	0.74	0.69	0.70	0.70	0.83	0.81	0.77	0.74	0.73
A..T	0.75	0.79	0.77	0.76	0.73	0.76	0.75	0.86	0.86	0.84	0.75	0.74
G..T	0.70	0.73	0.72	0.74	0.69	0.72	0.70	0.83	0.82	0.77	0.73	0.72
G..C	0.68	0.70	0.72	0.70	0.66	0.68	0.68	0.78	0.73	0.70	0.72	0.70
A..A	0.78	0.78	0.78	0.78	0.77	0.76	0.76	0.82	0.83	0.76	0.77	0.78
A..G	0.76	0.78	0.77	0.75	0.76	0.74	0.75	0.84	0.81	0.76	0.76	0.75
G..A	0.72	0.73	0.77	0.74	0.73	0.72	0.76	0.74	0.71	0.75	0.75	0.74
G..G	0.74	0.71	0.74	0.72	0.72	0.71	0.73	0.74	0.74	0.68	0.75	0.73
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G
max	0.82	0.83	0.84	0.81	0.78	0.80	0.80	0.86	0.86	0.84	0.81	0.80
mean	0.76	0.77	0.77	0.77	0.74	0.74	0.75	0.79	0.77	0.74	0.77	0.75
min	0.68	0.70	0.71	0.70	0.66	0.68	0.68	0.74	0.70	0.68	0.72	0.70
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G

X_m

Steps											Levels	
T..T	0.50	0.54	0.49	0.52	0.46	0.52	0.52	0.47	0.43	0.38	0.46	0.45
T..C	0.47	0.49	0.45	0.51	0.46	0.48	0.41	0.41	0.35	0.32	0.44	0.41
C..T	0.47	0.50	0.47	0.50	0.41	0.51	0.50	0.41	0.42	0.37	0.44	0.43
C..C	0.44	0.47	0.44	0.48	0.41	0.44	0.44	0.38	0.33	0.30	0.40	0.40
C..G	0.42	0.42	0.40	0.48	0.46	0.42	0.43	0.37	0.33	0.30	0.39	0.37
T..G	0.42	0.48	0.43	0.49	0.45	0.43	0.44	0.40	0.35	0.33	0.41	0.40
T..A	0.44	0.49	0.41	0.53	0.45	0.45	0.44	0.44	0.38	0.35	0.47	0.43
C..A	0.43	0.47	0.43	0.50	0.45	0.44	0.44	0.40	0.34	0.33	0.42	0.40
A..C	0.49	0.49	0.48	0.52	0.52	0.52	0.51	0.46	0.42	0.43	0.52	0.46
A..T	0.50	0.43	0.52	0.53	0.53	0.54	0.52	0.48	0.47	0.46	0.52	0.50
G..T	0.46	0.49	0.49	0.52	0.52	0.50	0.51	0.46	0.44	0.43	0.48	0.48
G..C	0.45	0.48	0.43	0.51	0.48	0.49	0.48	0.45	0.39	0.38	0.49	0.47
A..A	0.45	0.50	0.48	0.56	0.46	0.49	0.52	0.47	0.43	0.38	0.52	0.44
A..G	0.41	0.41	0.43	0.51	0.41	0.45	0.50	0.41	0.39	0.37	0.48	0.43
G..A	0.41	0.44	0.40	0.50	0.46	0.45	0.41	0.41	0.34	0.32	0.49	0.44
G..G	0.33	0.40	0.39	0.44	0.41	0.40	0.44	0.38	0.34	0.30	0.43	0.40
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G
max	0.50	0.54	0.52	0.56	0.53	0.54	0.52	0.48	0.47	0.46	0.52	0.50
mean	0.44	0.47	0.45	0.51	0.46	0.47	0.47	0.43	0.38	0.36	0.46	0.43
min	0.33	0.40	0.39	0.44	0.41	0.40	0.41	0.37	0.33	0.30	0.39	0.37
	GG	GA	AG	AA	GC	GT	AT	TA	TG	CG	A	G

Figure S4: Numerical data corresponding to figure 5. Average K⁺ population in the internal (I) and external (X) regions of the major (I_j, X_j) and minor (I_m, X_m) grooves are shown in the upper tables of each panel. See also caption of figure 5. The minimum, mean and maximum values for each column are given in the lower tables of each panel.

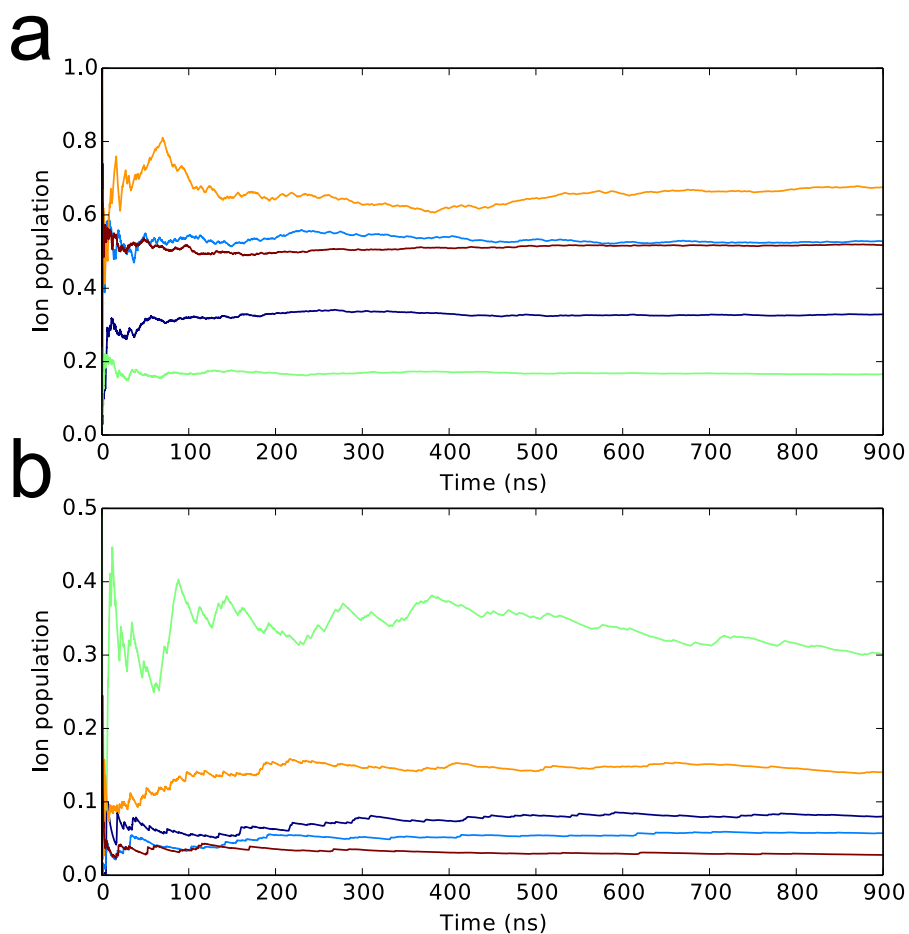


Figure S5: Convergence of ion populations. Cumulated ion populations as a function of simulation time within the major (a: Ij) and minor (b: Im) grooves are shown for five base-pair steps: AG (dark blue), GA (light blue), CG (green), GC (yellow) and GG (dark red). The values were measured at base-pair steps 9-10 and 10-11 of the AGAG oligomer, steps 9-10 and 10-11 of the CGCG oligomer and step 9-10 of the GGGG oligomer.

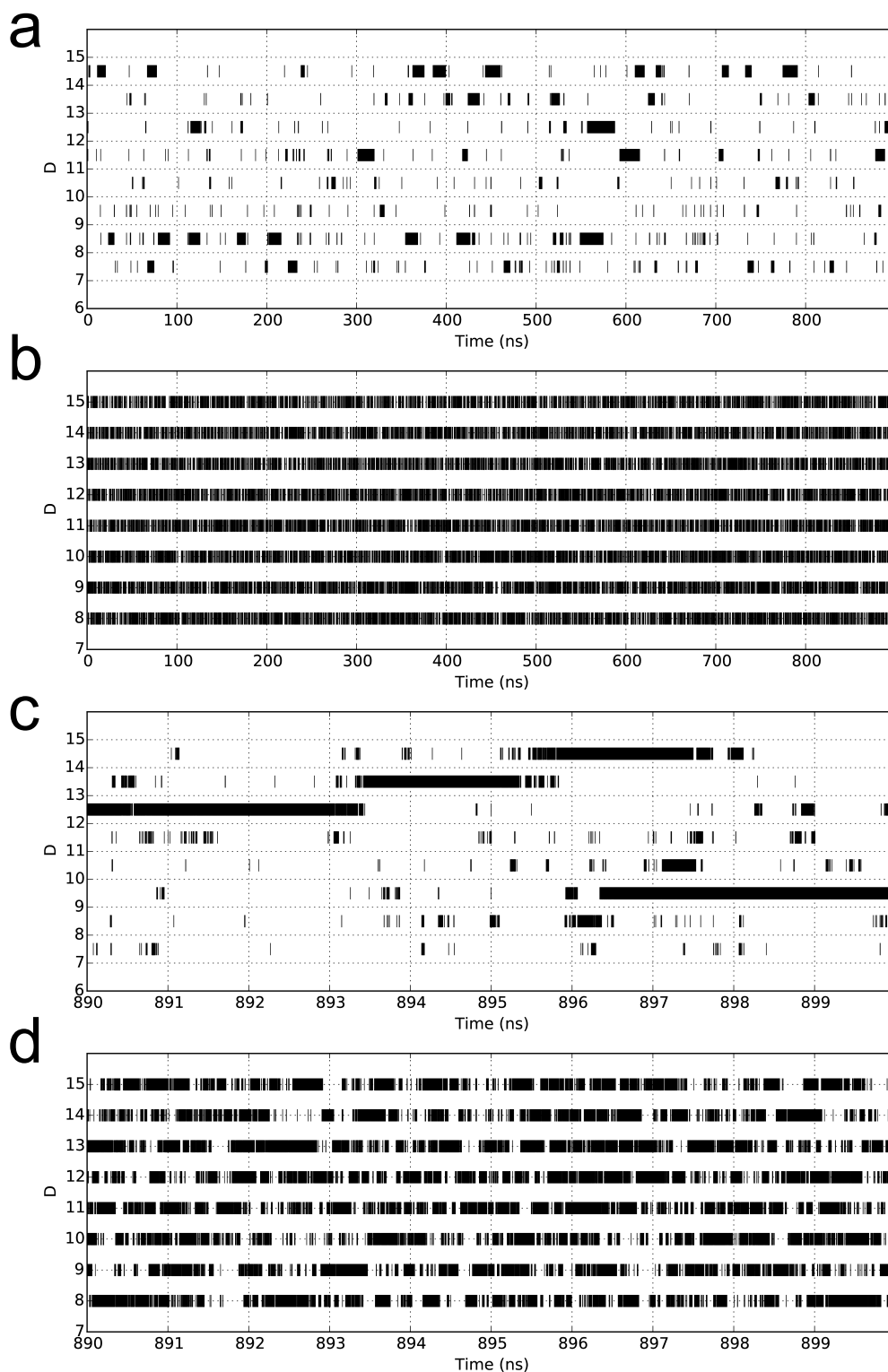


Figure S6. Time-dependent ion occupancies. Ion binding at eight consecutive base pair steps in minor groove of the central part of the AAAA oligomer (a, c) and at eight consecutive base pairs in the major groove of the central part of the GGGG oligomer (b, d). In panels (a) and (b), black vertical lines indicate ion binding during at least 75 ps within non-overlapping 100 ps windows, plotted for the full-length 900 ns trajectories. In panels (c) and (d), black vertical lines indicate ion binding at each snapshot (every 1 ps), plotted for the last 10 ns of the simulations.