Supporting information

Structure, stiffness and substates of the Dickerson-Drew dodecamer

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	System	Tilt	Roll	Twist	Shift	Slide	Rise
CG	KCl_Dg	1.13(0.07)	9.36(0.12)	24.62(0.41)	0.05(0.00)	-0.13(0.00)	3.07(0.02)
	Na_Bsc	1.33(0.14)	8.29(0.06)	25.49(0.38)	0.08(0.03)	-0.12(0.02)	3.10(0.00)
	KCl_JC	1.45(0.23)	8.30(0.38)	23.04(1.55)	0.11(0.01)	-0.01(0.07)	2.98(0.02)
	NMR	2.00(0.41)	6.58(0.92)	33.13(0.73)	0.10(0.10)	-0.08(0.09)	3.42(0.03)
GA	KCl_Dg	0.25(0.04)	2.63(0.07)	36.65(0.26)	-0.29(0.02)	-0.24(0.03)	3.44(0.00)
	Na_Bsc	0.07(0.04)	2.91(0.16)	36.04(0.42)	-0.35(0.03)	-0.20(0.04)	3.46(0.00)
	KCl_JC	0.20(0.15)	1.96(0.08)	38.97(0.26)	-0.45(0.05)	-0.07(0.06)	3.47(0.02)
	NMR	-0.46(0.29)	5.45(0.13)	36.67(0.14)	-0.38(0.05)	-0.17(0.05)	3.20(0.02)
AA	KCl_Dg	-2.28(0.00)	1.82(0.16)	35.08(0.01)	-0.08(0.00)	-0.58(0.01)	3.35(0.00)
	Na_Bsc	-2.22(0.19)	2.21(0.02)	34.70(0.06)	-0.07(0.01)	-0.67(0.02)	3.38(0.00)
	KCl_JC	-2.19(0.02)	1.38(0.08)	35.97(0.03)	-0.05(0.01)	-0.54(0.01)	3.37(0.01)
	NMR	-0.55(0.20)	-0.13(0.59)	37.87(0.17)	-0.46(0.02)	-0.23(0.03)	3.10(0.02)
AT	KCl_Dg	0.09(0.01)	-0.73(0.01)	31.92(0.02)	0.00(0.01)	-0.97(0.00)	3.33(0.00)
	Na_Bsc	-0.03(0.01)	-0.40(0.07)	32.19(0.04)	0.00(0.01)	-1.06(0.00)	3.35(0.00)
	KCl_JC	0.04(0.02)	-1.82(0.11)	31.92(0.06)	-0.01(0.02)	-0.94(0.01)	3.30(0.01)
	NMR	0.01(0.06)	-2.61(0.53)	34.59(0.17)	-0.01(0.02)	-0.63(0.03)	2.97(0.06)
TT	KCl_Dg	2.22(0.03)	1.68(0.20)	35.28(0.19)	0.11(0.01)	-0.57(0.01)	3.36(0.00)
	Na_Bsc	2.33(0.04)	2.19(0.02)	34.31(0.08)	0.06(0.00)	-0.67(0.01)	3.37(0.00)
	KCl_JC	2.16(0.01)	1.44(0.03)	36.12(0.03)	0.05(0.02)	-0.53(0.01)	3.38(0.00)
	NMR	0.64(0.32)	-0.04(0.56)	37.90(0.15)	0.44(0.03)	-0.20(0.03)	3.10(0.01)
TC	KCl_Dg	-0.43(0.05)	2.46(0.15)	36.14(0.07)	0.24(0.01)	-0.28(0.02)	3.46(0.00)
	Na_Bsc	0.02(0.04)	2.81(0.14)	36.28(0.08)	0.41(0.00)	-0.21(0.00)	3.44(0.00)
	KCl_JC	0.09(0.01)	2.10(0.07)	38.90(0.66)	0.51(0.08)	0.01(0.02)	3.45(0.00)
	NMR	0.33(0.15)	5.42(0.37)	36.71(0.20)	0.37(0.05)	-0.14(0.07)	3.21(0.01)
CG	KCl_Dg	-1.21(0.19)	8.53(0.03)	25.64(0.64)	-0.04(0.02)	-0.06(0.00)	3.07(0.00)
	Na_Bsc	-1.21(0.11)	8.44(0.30)	25.34(0.91)	-0.13(0.03)	-0.16(0.03)	3.11(0.02)
	KCl_JC	-1.78(0.11)	7.83(0.07)	22.47(1.40)	-0.11(0.06)	-0.06(0.04)	2.98(0.04)
	NMR	-1.90(0.33)	6.54(0.87)	33.22(0.67)	-0.09(0.07)	-0.05(0.09)	3.43(0.01)

Table S1: Average values of inter-basepair (or step) coordinates obtained from the simulated trajectories and from the NMR experiment. Each block corresponds to a particular step within the inner octamer of the Dickerson-Drew dodecamer. All the numbers are supplemented with their error estimates. In the case of MD simulations the errors were estimated as the average of the absolute differences between the whole trajectory values and the values obtained from the first and second halves of the trajectory. For NMR data, the standard deviations of the values for the five NMR models are shown. The MD data were calculated from the trajectories filtered to keep the WW end states only.

	System	Buckle	Propeller	Opening	Shear	Stretch	Stagger
C	KCl_Dg	-3.25(0.63)	-4.17(0.43)	-0.68(0.04)	0.14(0.01)	-0.06(0.00)	0.16(0.01)
	Na_Bsc	-2.26(0.49)	-3.97(0.14)	-0.89(0.01)	0.10(0.00)	-0.05(0.00)	0.16(0.00)
	KCl_JC	-3.73(1.27)	-2.57(0.40)	-0.52(0.07)	0.12(0.01)	-0.05(0.00)	0.23(0.01)
	NMR	-3.69(0.43)	-14.18(1.53)	0.81(1.09)	0.41(0.08)	-0.47(0.04)	-0.05(0.11)
G	KCl_Dg	8.51(0.21)	-7.81(0.12)	-0.03(0.01)	-0.13(0.00)	-0.05(0.00)	0.03(0.00)
	Na_Bsc	8.69(0.52)	-6.96(0.08)	0.09(0.01)	-0.12(0.00)	-0.04(0.00)	0.04(0.01)
	KCl_JC	11.98(0.36)	-7.58(1.17)	0.37(0.10)	-0.13(0.01)	-0.04(0.00)	0.09(0.02)
	NMR	0.32(0.35)	-13.36(1.10)	-1.26(0.98)	-0.19(0.08)	-0.39(0.02)	0.01(0.04)
A	KCl_Dg	4.81(0.30)	-17.76(0.13)	0.31(0.05)	0.11(0.00)	0.01(0.00)	-0.08(0.00)
	Na_Bsc	5.20(0.39)	-17.24(0.10)	-0.15(0.21)	0.14(0.01)	0.02(0.00)	-0.09(0.00)
	KCl_JC	6.81(0.61)	-19.20(0.37)	-0.19(0.06)	0.12(0.00)	0.01(0.00)	-0.08(0.01)
	NMR	-3.89(0.31)	-19.64(0.14)	-1.13(0.76)	-0.20(0.05)	-0.27(0.05)	-0.18(0.04)
A	KCl_Dg	0.92(0.08)	-17.98(0.17)	0.30(0.04)	0.11(0.00)	0.01(0.00)	0.09(0.00)
	Na_Bsc	0.97(0.17)	-17.91(0.16)	0.29(0.02)	0.11(0.00)	0.01(0.00)	0.05(0.00)
	KCl_JC	0.90(0.47)	-19.94(0.01)	-0.34(0.12)	0.14(0.00)	0.01(0.00)	0.08(0.00)
	NMR	-1.81(0.83)	-22.94(0.17)	-2.76(0.55)	-0.06(0.01)	-0.23(0.06)	-0.24(0.05)
T	KCl_Dg	-0.87(0.02)	-18.04(0.16)	0.34(0.10)	-0.11(0.00)	0.01(0.00)	0.08(0.00)
	Na_Bsc	-1.19(0.12)	-17.75(0.14)	0.22(0.05)	-0.11(0.00)	0.01(0.00)	0.05(0.00)
	KCl_JC	-1.48(0.29)	-19.97(0.06)	-0.35(0.08)	-0.14(0.00)	0.01(0.00)	0.07(0.00)
	NMR	1.76(0.77)	-22.96(0.10)	-2.68(0.64)	0.07(0.02)	-0.24(0.06)	-0.24(0.05)
T	KCl_Dg	-4.85(0.10)	-17.86(0.02)	0.36(0.27)	-0.11(0.01)	0.01(0.00)	-0.08(0.01)
	Na_Bsc	-5.12(0.25)	-16.89(0.05)	0.08(0.06)	-0.13(0.00)	0.02(0.00)	-0.09(0.00)
	KCl_JC	-7.63(0.41)	-18.89(0.10)	-0.16(0.08)	-0.12(0.00)	0.01(0.00)	-0.07(0.01)
	NMR	3.97(0.47)	-19.47(0.35)	-1.00(0.99)	0.20(0.05)	-0.27(0.06)	-0.19(0.05)
C	KCl_Dg	-8.83(0.01)	-7.43(0.29)	0.08(0.05)	0.12(0.00)	-0.04(0.00)	0.03(0.01)
	Na_Bsc	-8.14(0.26)	-7.15(0.39)	0.13(0.12)	0.11(0.01)	-0.04(0.00)	0.04(0.00)
	KCl_JC	-11.95(0.44)	-6.86(0.38)	0.32(0.06)	0.13(0.00)	-0.04(0.00)	0.06(0.01)
	NMR	-0.34(0.19)	-13.31(1.03)	-1.33(0.92)	0.18(0.07)	-0.39(0.02)	0.03(0.03)
G	KCl_Dg	3.47(0.17)	-2.34(0.44)	-0.76(0.01)	-0.14(0.00)	-0.05(0.00)	0.16(0.01)
	Na_Bsc	2.19(0.66)	-3.80(0.11)	-0.71(0.02)	-0.11(0.00)	-0.05(0.00)	0.15(0.01)
	KCl_JC	4.00(1.02)	-2.14(1.21)	-0.58(0.27)	-0.11(0.01)	-0.06(0.00)	0.22(0.03)
	NMR	3.72(0.53)	-14.32(1.57)	0.77(0.88)	-0.40(0.07)	-0.46(0.03)	-0.05(0.08)

Table S2: Average values of intra-basepair coordinates obtained from the simulated systems and from the NMR experiment. For detailed description see Tab. S1.

KL divergence (TT state)			
	KCl_Dg	KCl_JC	Na_Bsc
KCl_Dg	0.59, 0.62	-	1.32
KCl_JC	-	-	-
Na_Bsc	1.32	-	0.47, 0.39

Riemann distance (TT state)			
	KCl_Dg	KCl_JC	Na_Bsc
KCl_Dg	0.83, 0.87	-	1.86
KCl_JC	-	-	-
Na_Bsc	1.86	-	0.66, 0.55

Table S3: KL divergences and Riemann distances between stiffness matrices computed from the whole trajectories and from their halves (diagonal entries), and between stiffness matrices from different simulations. Only the TT end state is considered. See Table 2 in the main text for the WW state values.

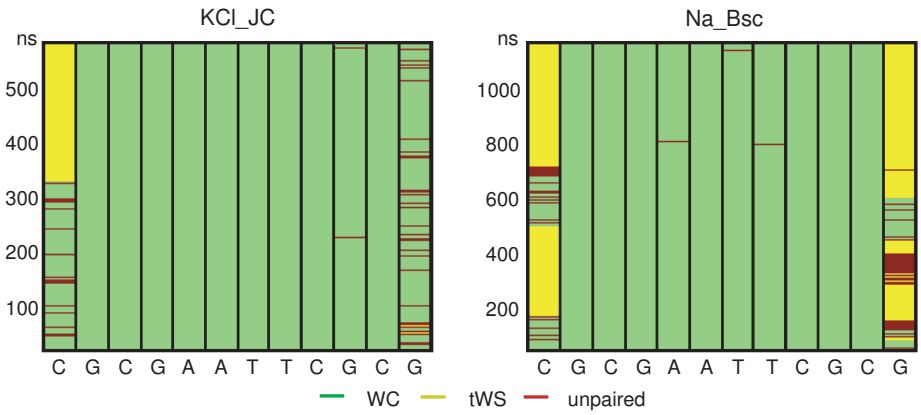

Figure S1: Time evolution of base pairing in the KCl_JC and Na_Bsc simulations. WC: Watson-Crick pairs, tWS: trans Watson-Crick/Sugar Edge pairs. See Figure 1 in the main text for the KCl_Dg data and for further details.

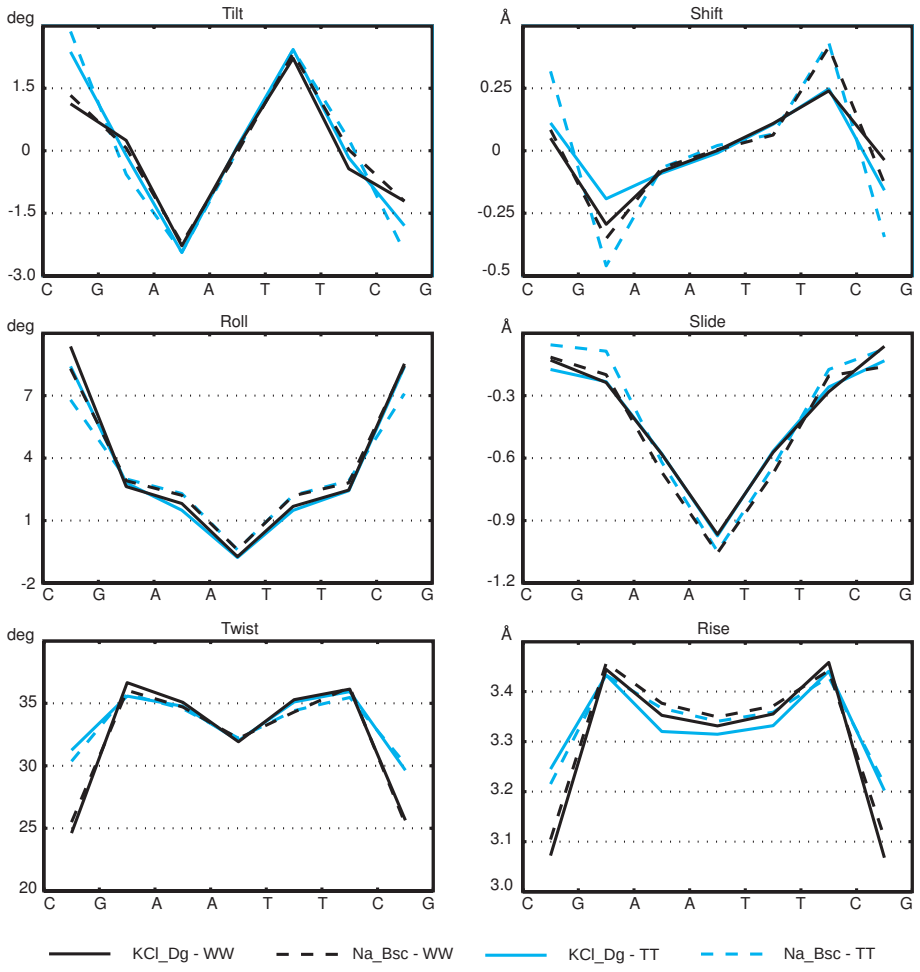

Figure S2: Mean values of the step coordinates for the WW and TT end states. Only the inner octamer is shown. The differences between the WW and TT values are small, except for the CG steps.

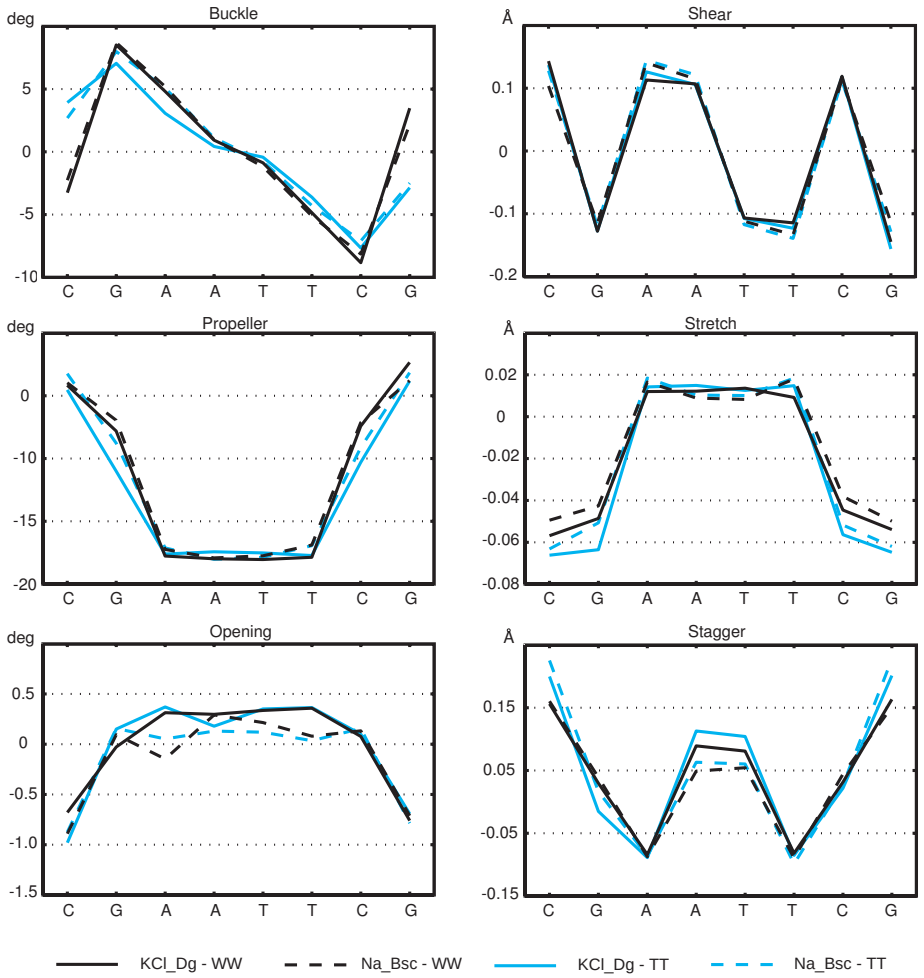

Figure S3: Mean values of the intra-basepair coordinates for the WW and TT end states. Only the inner octamer is shown. The WW and TT values are very close, perhaps except the outermost C.G pairs of the octamer.

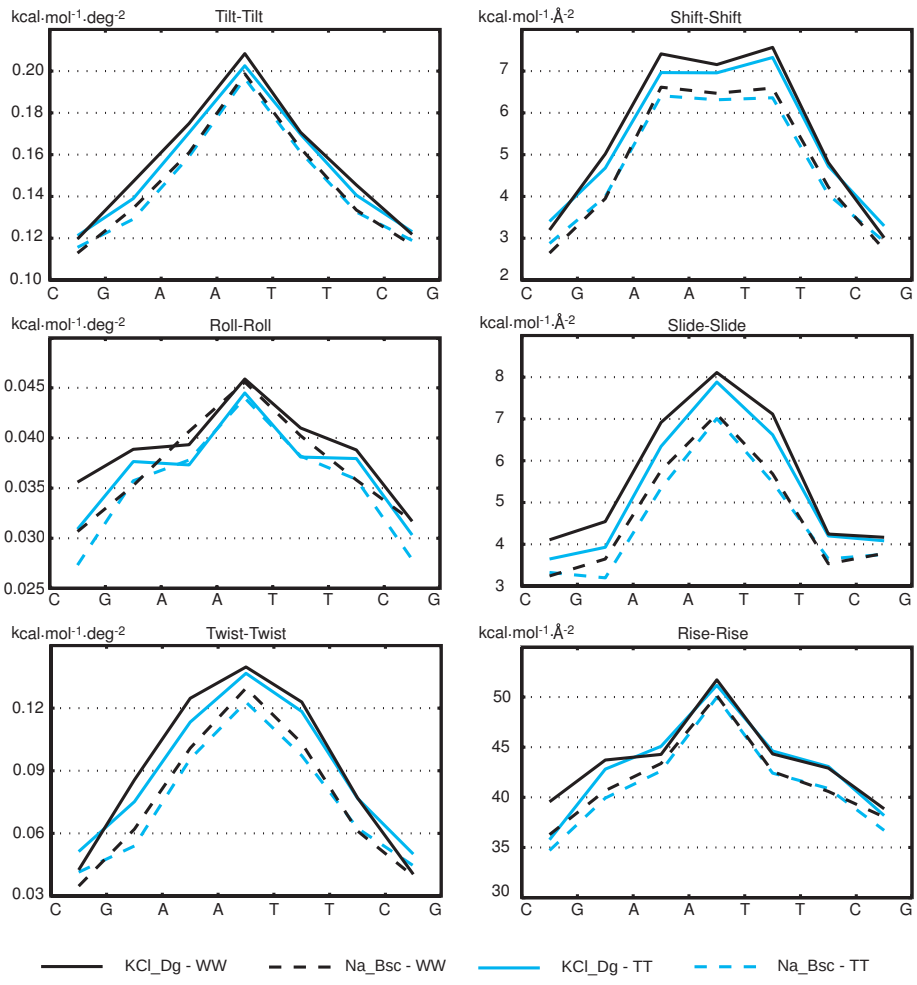

Figure S4: Diagonal entries of the stiffness matrix corresponding to the step coordinates, obtained for the WW and TT end states. The stiffness matrix is only computed for the inner octamer. The WW/TT differences are visible, but are mostly smaller than the differences between individual simulations.

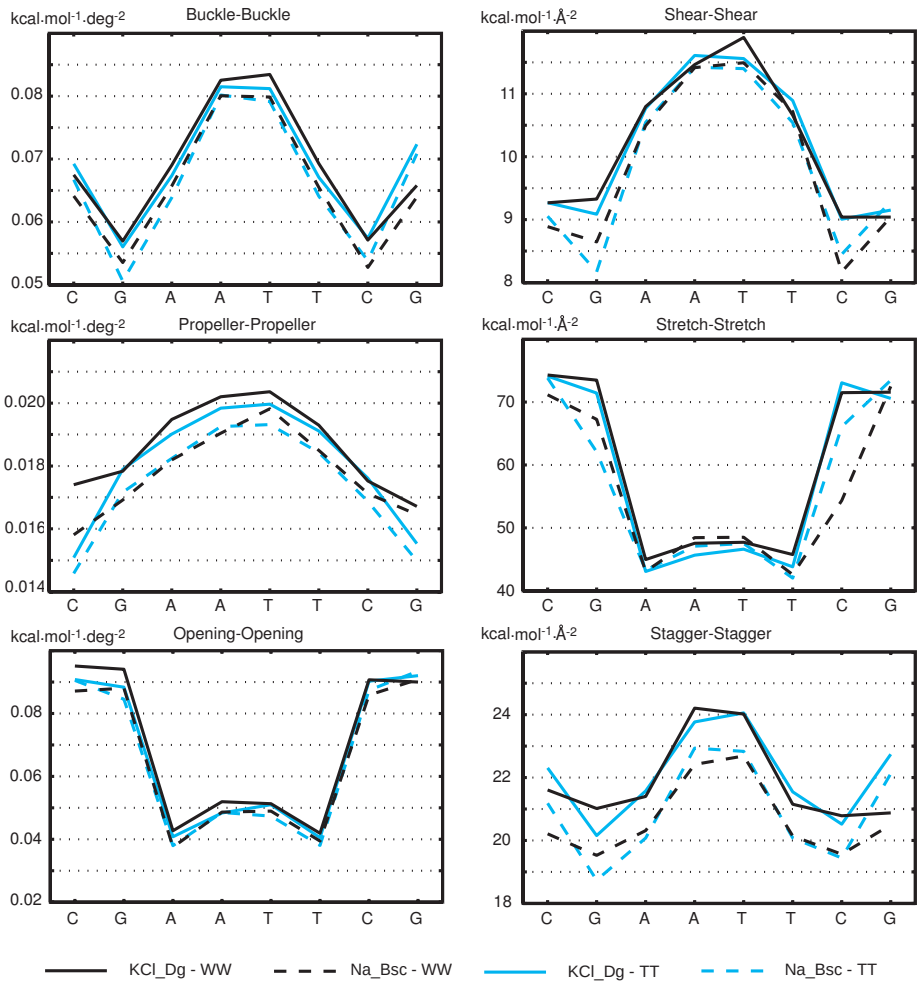

Figure S5: Diagonal entries of the stiffness matrix corresponding to the intra-basepair coordinates, obtained for the WW and TT end states. The stiffness matrix is only computed for the inner octamer. Differences are in general small.

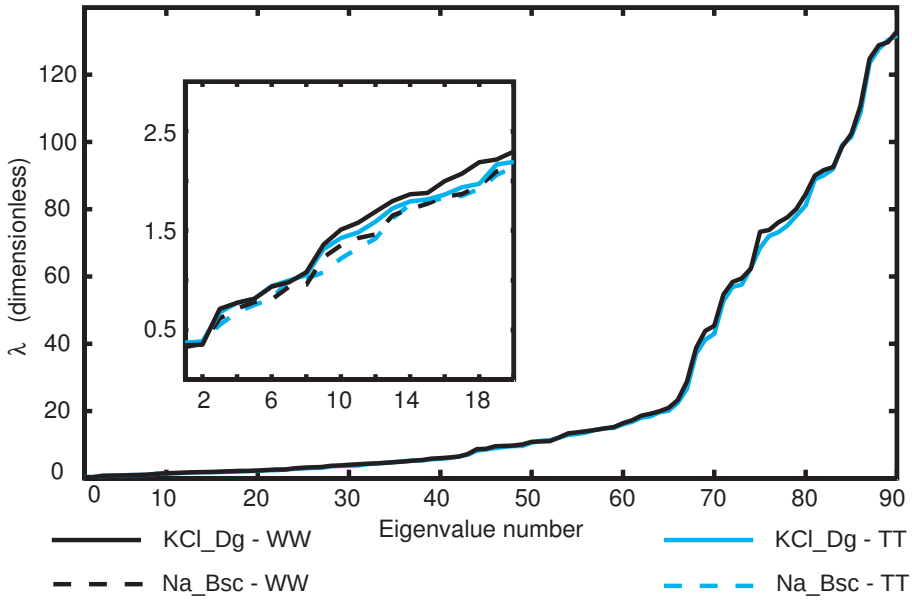

Figure S6: Eigenvalues of the stiffness matrix in its reduced form, computed for the WW and TT end states. Differences are rather small. Compare with Figure 12 in the main text.

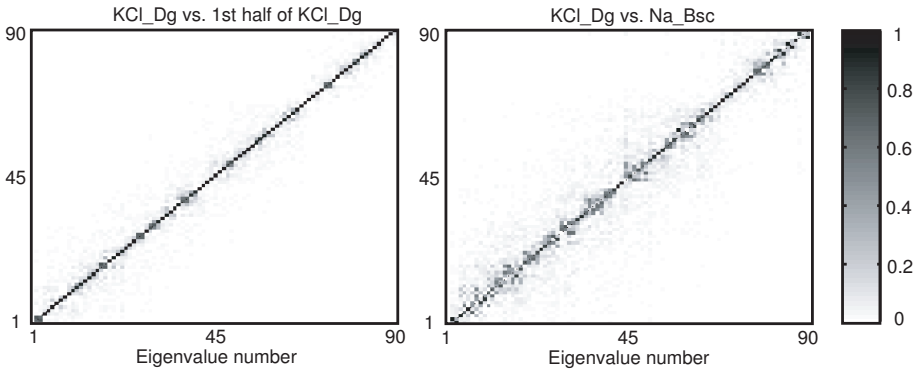

Figure S7: Scalar products between the stiffness matrix eigenvectors of the KCl_Dg and Na_Bsc simulations in the TT state. Just as for the WW state (Figure 13 in the main text), the eigenvectors from the whole trajectory and its first half are closer to each other than the eigenvectors of the two simulations.