Supporting information

Sodium and magnesium ion location at the backbone and at the nucleobase of RNA: ab initio molecular dynamics in water solution

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Supporting information contains Tables S1 and S2 and Figures S1-S11.

Table S1. Average number (n) of oxygen atoms from the first coordination shell of Na^+ or Mg^{2+} ions and percentage of time spent by the ion with different numbers n of coordinated oxygen atoms. Empty cells indicate that no time was spent in the given configuration.

ssRNA	Cation	n±SD	n = 3	n = 4	n = 5	n = 6	n = 7	n = 8
CC	Na^+ 1 bound	4.9 ± 0.7	0.02	27.76	55.14	16.67	0.40	0.01
	Na^+ 2 bound	5.2 ± 0.7	0.19	13.14	54.25	31.25	1.06	0.11
CC	Na^+ 1 solvated	5.4 ± 0.6		3.32	55.27	40.69	0.71	0.01
	Na^+ 2 solvated	5.6 ± 0.6		4.08	32.86	58.39	4.54	0.13
GC	Na^+ 1 bound	4.7 ± 0.5	0.48	32.58	63.70	3.18	0.06	
	Na^+ 2 bound	5.4 ± 0.6	0.13	4.13	51.60	41.90	2.24	
CC	Mg^{2+} bound	6.0 ± 0.1			0.72	99.28		
CC	Mg^{2+} solvated	6.0 ± 0.0				100		
GC	Mg^{2+} bound	6.0 ± 0.0			0.13	99.87		

Table S2. Percentage of time spent by the RNA backbone in gg, gt, tg or tt conformation. Empty cells indicate that no time was spent in the given conformation.

ssRNA	Cations	gg	gt	tg	tt
CC	2 Na^+ bound	99.981		0.019	
CC	2 Na^+ solvated	97.719		2.281	
GC	2 Na^+ bound	92.929		7.071	
CC	$Mg2^+$ bound	99.970		0.030	
CC	$Mg2^+$ solvated	99.924		0.076	
GC	$Mg2^+$ bound	99.233	0.157	0.610	

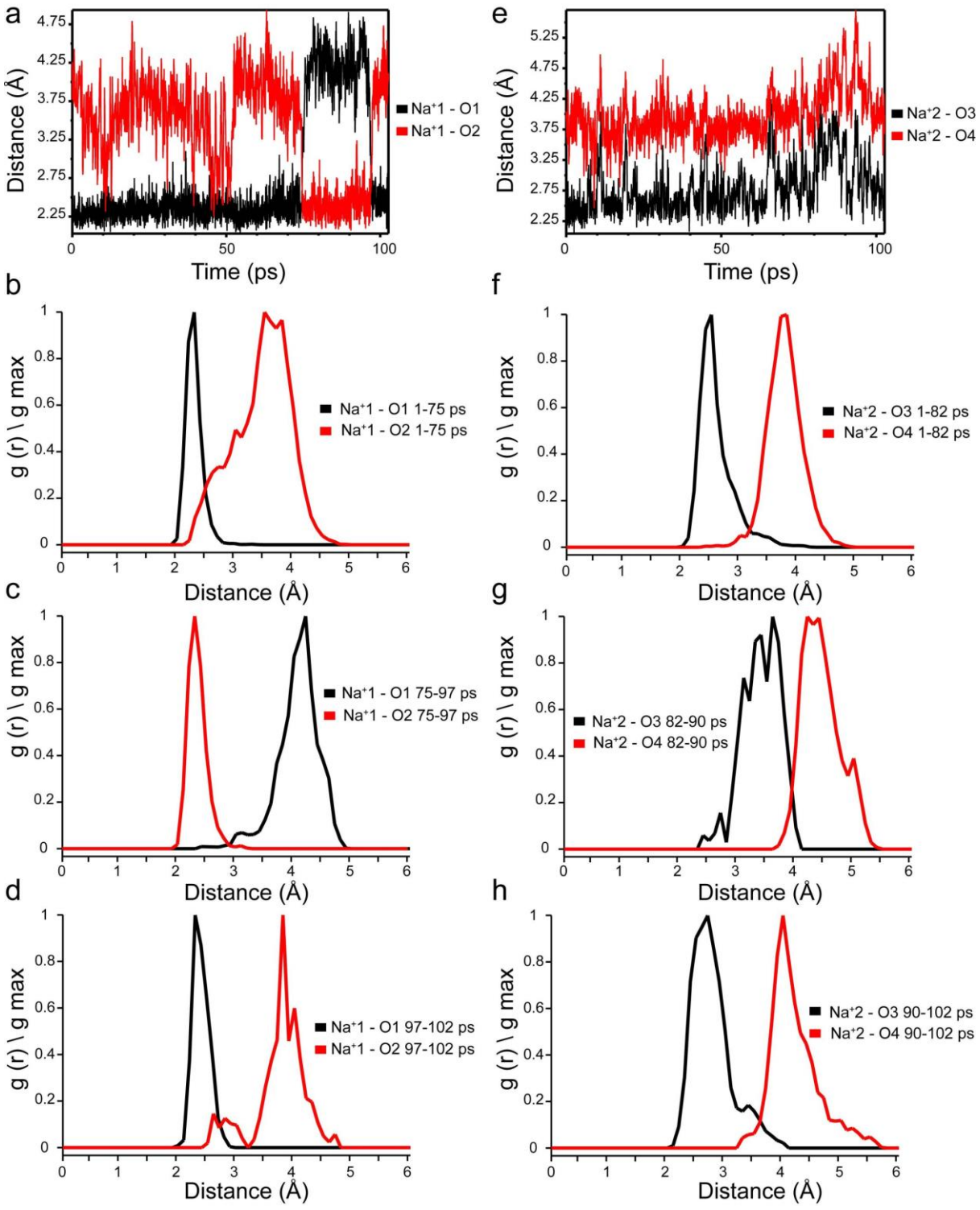

Figure S1. Dynamics of Na^+1–O1 and Na^+1–O2 distances from the ion to the O atom of the PO_4 group (a); Na^+2–O3 and Na^+2–O4 (e); RDFs for the corresponding distances Na^+1–O1 and Na^+1–O2 (b), (c) and (d); RDFs for the corresponding distances Na^+2–O3 and Na^+2–O4 (f), (g) and (h). All graphics are derived from the CC $2Na^+$ simulation with two bound sodium ions.

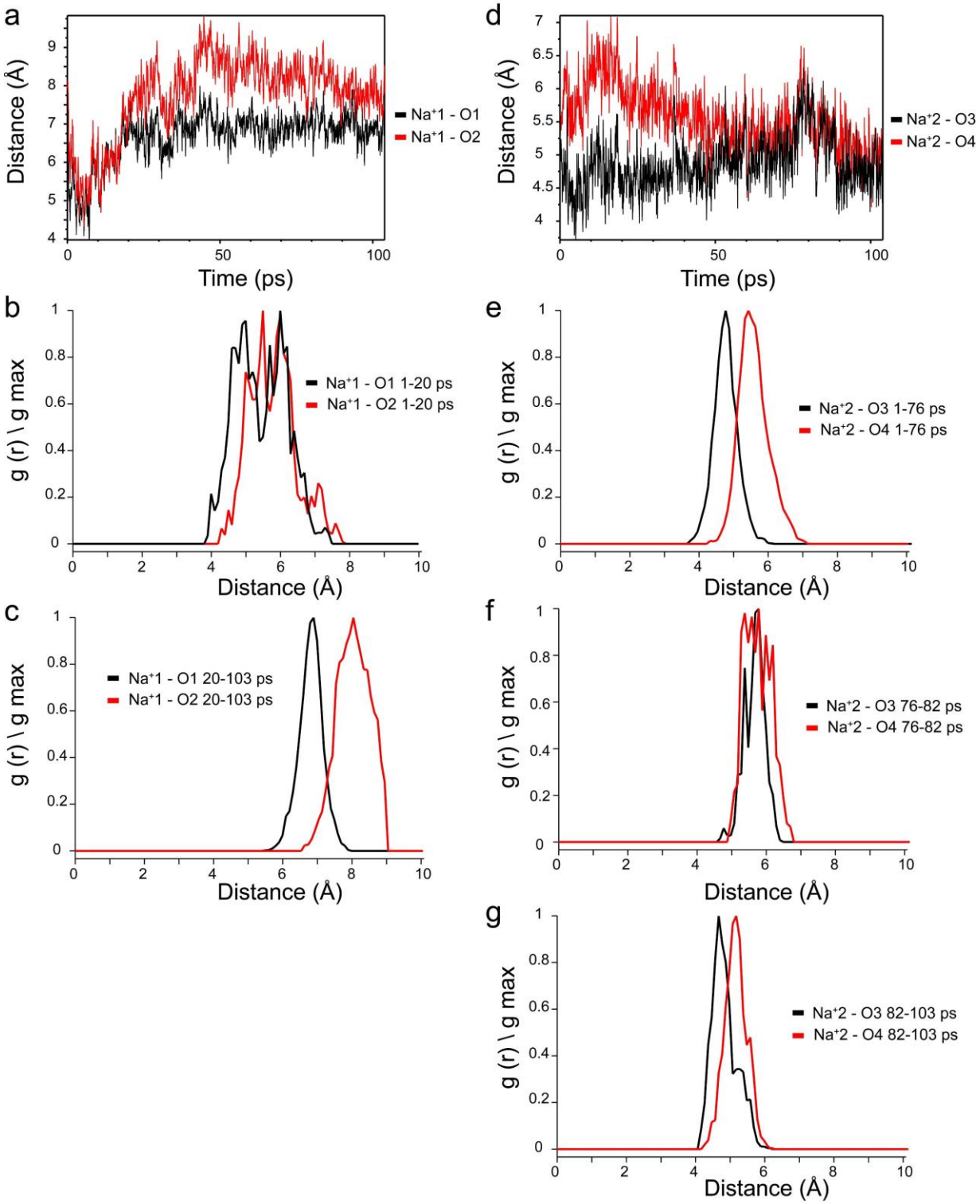

Figure S2: Dynamics of Na^+1–O1 and Na^+1–O2 distances from the ion to the O atom of the PO_4 group (a); Na^+2–O3 and Na^+2–O4 (d); RDFs for the corresponding distances Na^+1–O1 and Na^+1–O2 (b), (c); RDFs for the corresponding distances Na^+2–O3 and Na^+2–O4 (e), (f) and (g). All graphics are derived from the CC $2Na^+$ simulation with two solvated sodium ions.

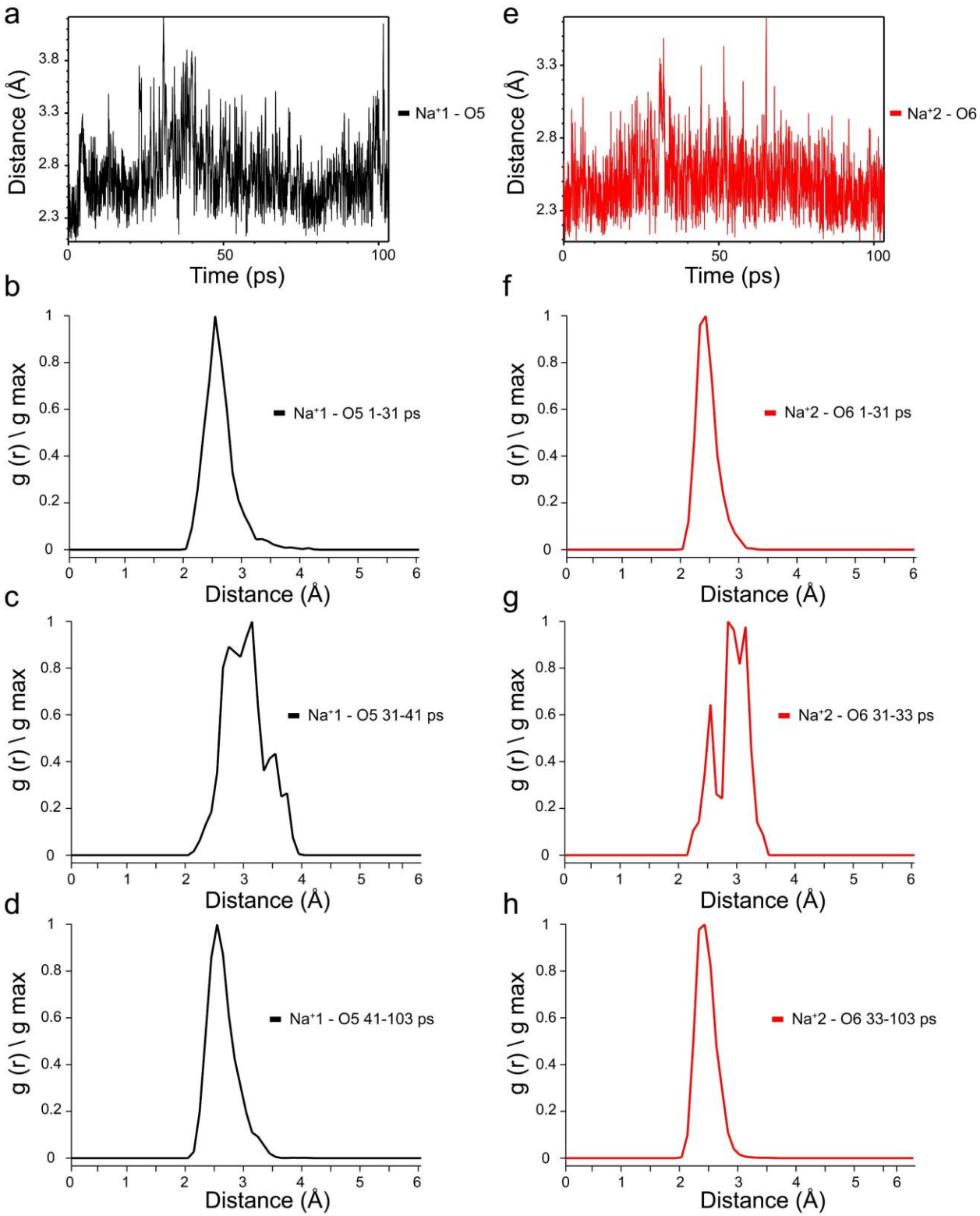

Figure S3. Dynamics of Na^+1–O5 distance from the ion to the O atom of the PO_4 group (a); Na^+2–O6 (e); RDFs for the corresponding distance Na^+1–O5 (b), (c), (d); RDFs for the corresponding distance Na^+2–O6 (f), (g), (h). All graphics are derived from the GC $2Na^+$ simulation with two bound sodium ions.

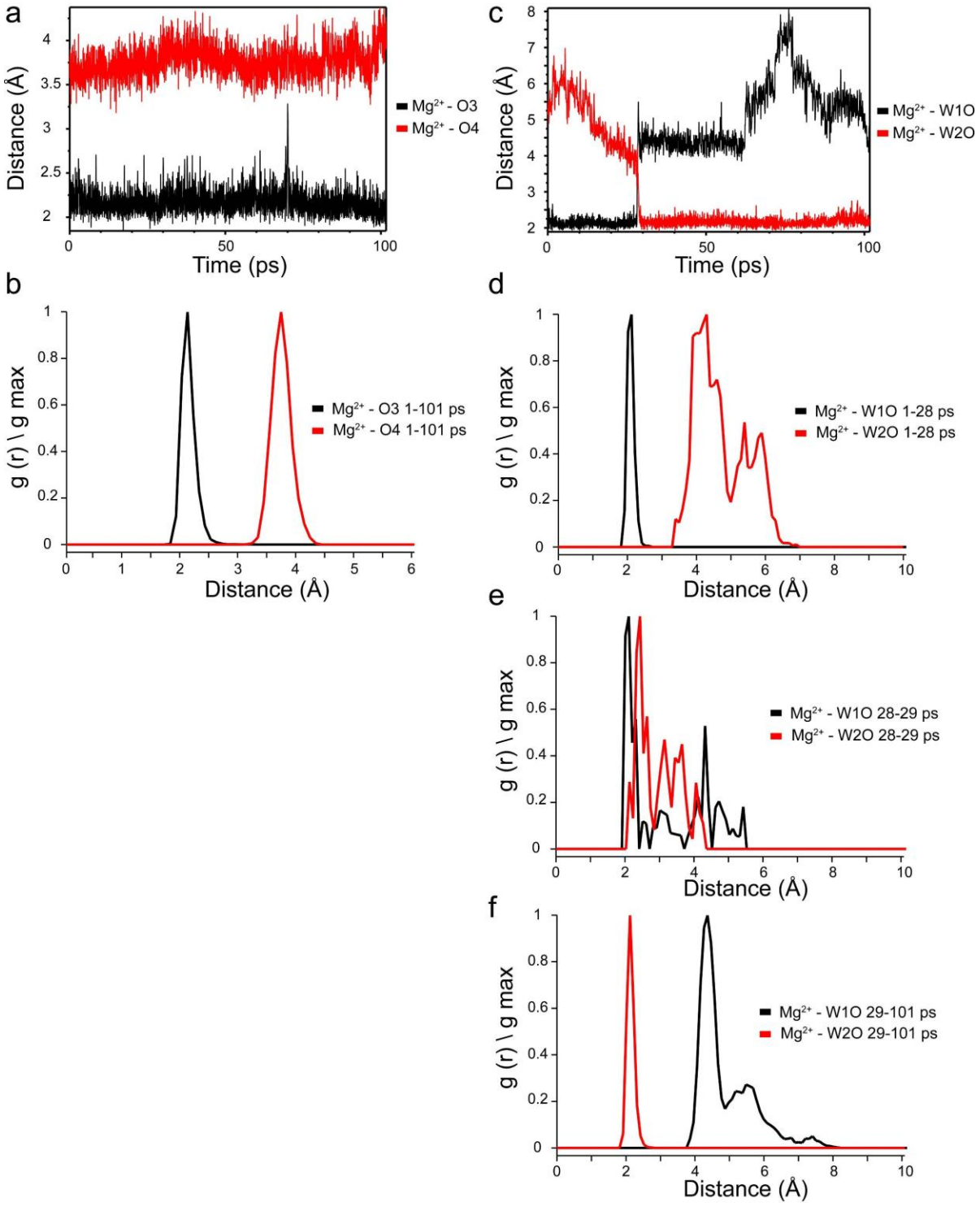

Figure S4. Dynamics of Mg^{2+}–O3 and Mg^{2+}–O4 distances from the ion to the O atom of the PO_4 group (a); Mg^{2+}–W1O, Mg^{2+}–W2O (c); RDFs for the corresponding distances Mg^{2+}–O3 and Mg^{2+}–O4 (b); RDFs for the corresponding distances Mg^{2+}–W1O and Mg^{2+}–W2O (d), (e) and (f). All graphics are derived from the CC Mg^{2+} simulation with one bound magnesium ion.

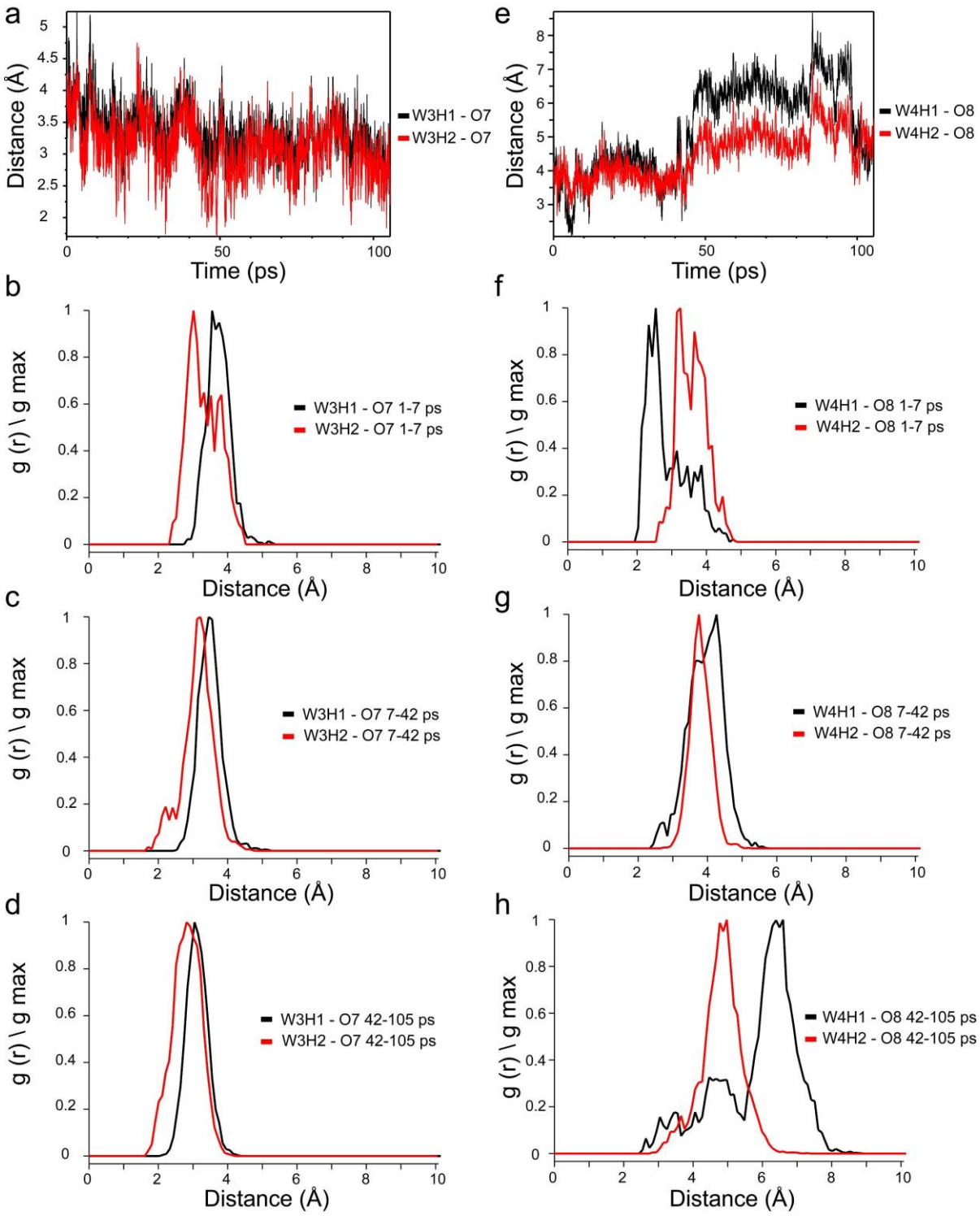

Figure S5. Dynamics of W3H1–O7 and W3H2–O7 distances from the H atom of the water molecule to the O atom of the PO_4 group (a); W4H1–O8 and W4H2–O8 (e); RDFs for the corresponding distances W3H1–O7 and W3H2–O7 (b), (c) (d); RDFs for the corresponding distances W4H1–O8 and W4H2–O8 (f), (g) and (h). All graphics are derived from the CC Mg^{2+} simulation with one solvated magnesium ion.

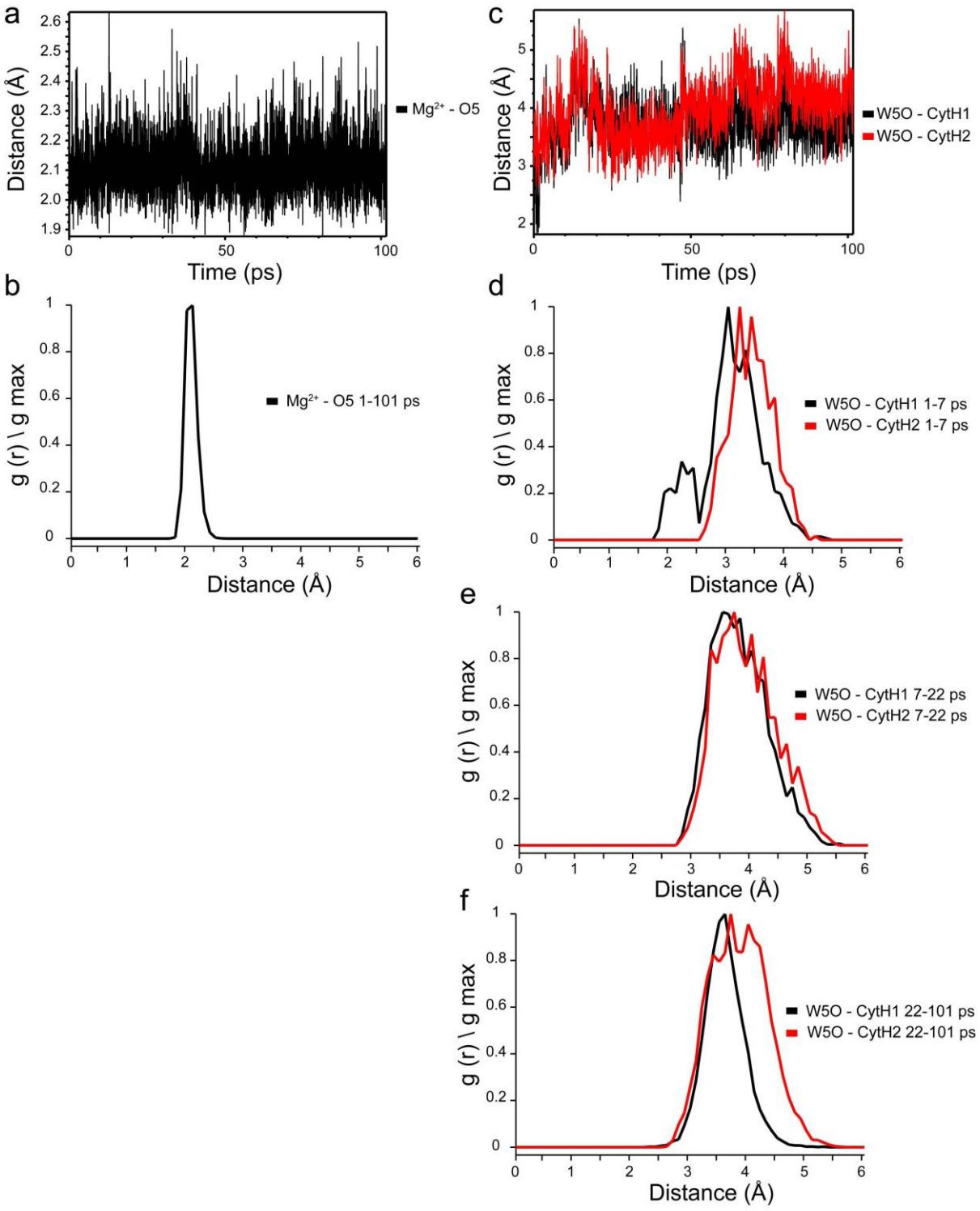

Figure S6. Dynamics of Mg^{2+}–O5 distance from the ion to the O atom of cytosine (see Figure 2) (a); W5O–CytH1 and W5O–CytH1, from water oxygen atom to the NH_2 group of cytosine (c); RDFs for the corresponding distance Mg^{2+}–O5 (b); RDFs for the corresponding distances W5O–CytH1 and W5O–CytH1 (d), (e) and (f). All graphics are derived from the GC Mg^{2+} simulation with one bound magnesium ion.

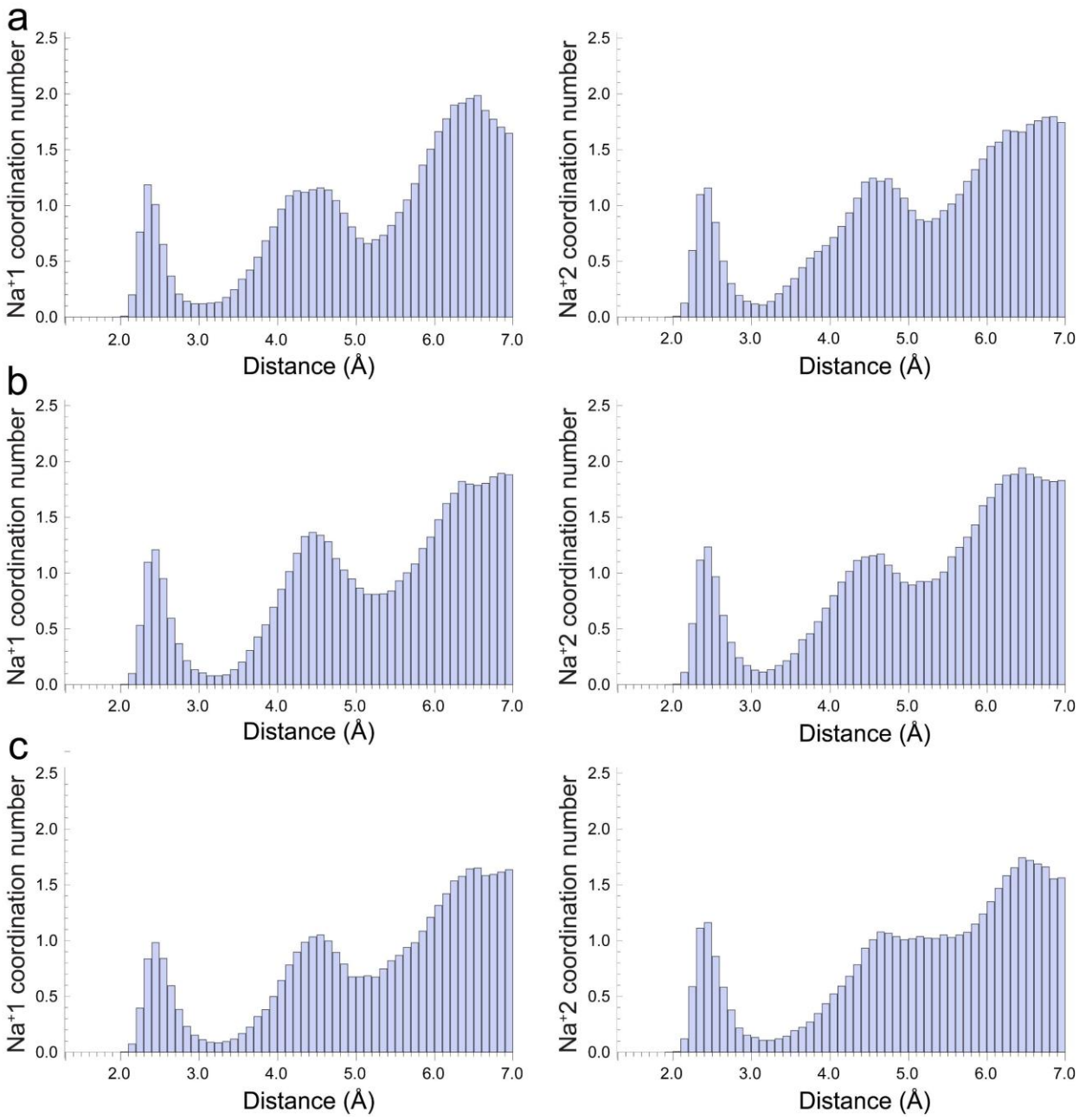

Figure S7: Histograms of the oxygen O atoms occurrence in the solvation shells of Na^+1 and Na^+2 ions in (a) CC $2Na^+$ simulation with two bound sodium ions, (b) CC $2Na^+$ simulation with two solvated sodium ions, and (c) GC $2Na^+$ simulation with two bound sodium ions.

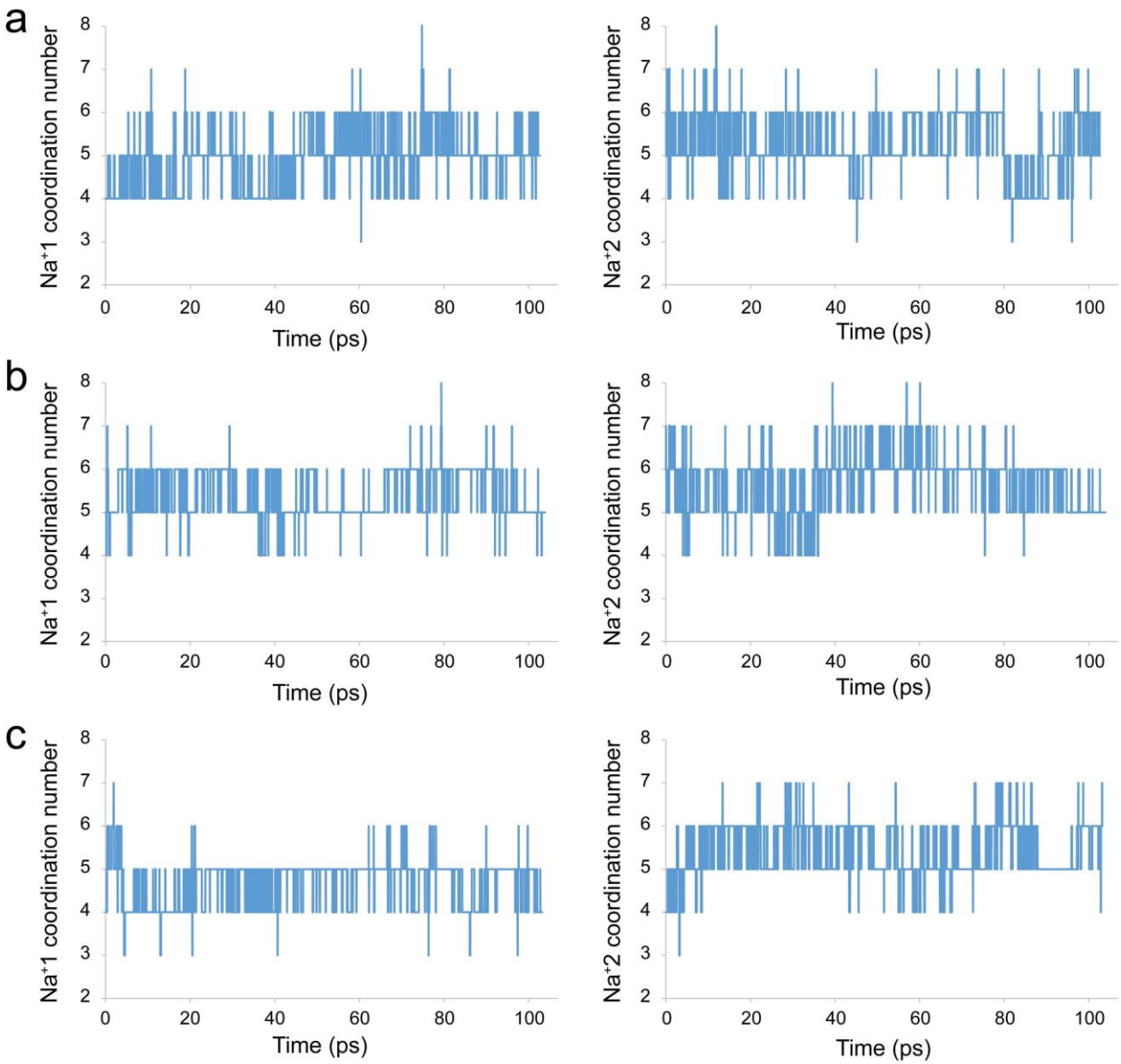

Figure S8. Dynamics of Na^+1 and Na^+2 coordination numbers with cut-off radius r = 3:2 Å in (a) CC $2Na^+$ simulation with two bound sodium ions; (b) CC $2Na^+$ simulation with two solvated sodium ions; and (c) GC $2Na^+$ simulation with two bound sodium ions.

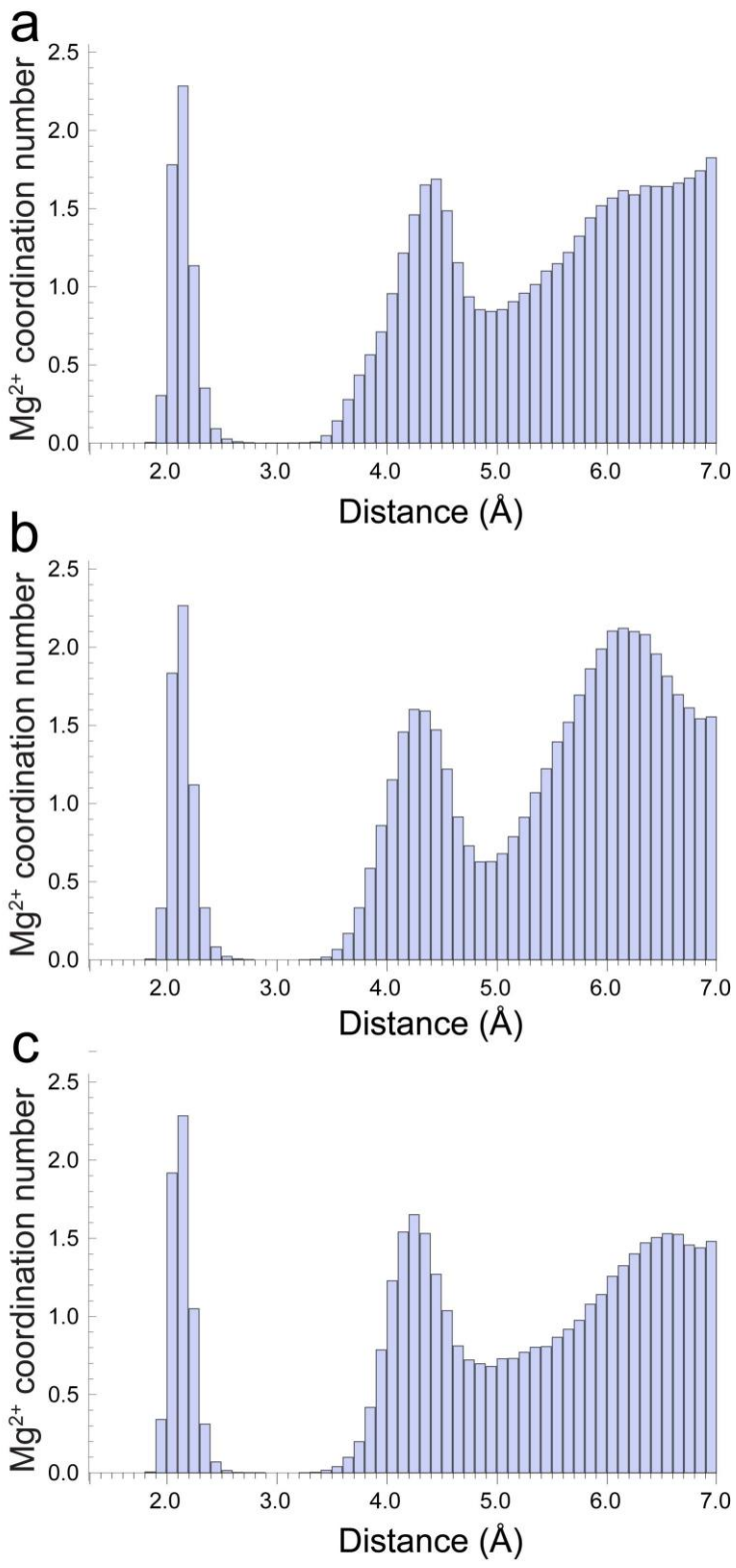

Figure S9. Histograms of the oxygen O atoms occurrence in the solvation shell of Mg^{2+} ion in (a) CC Mg^{2+} simulation with one bound magnesium ion; (b) CC Mg^{2+} simulation with one solvated magnesium ion; and (c) GC Mg^{2+} simulation with one bound magnesium ion.

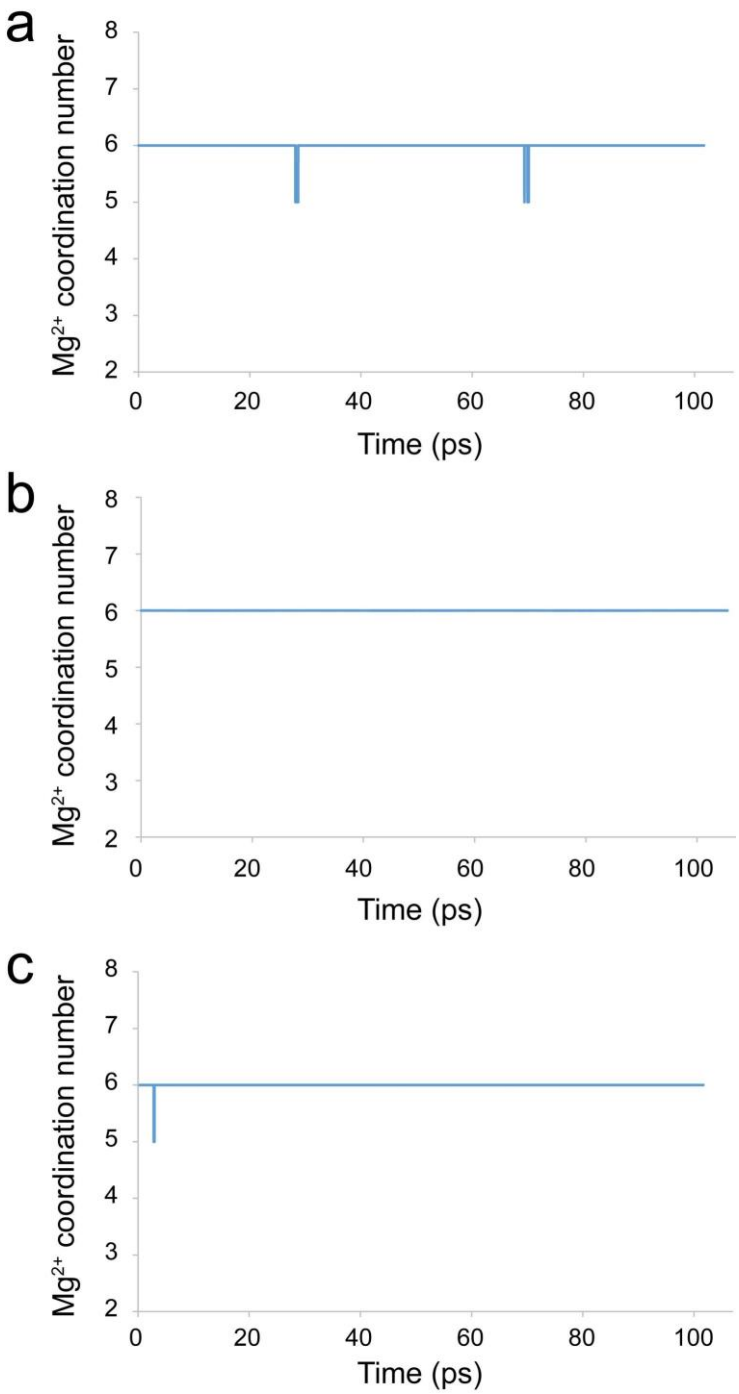

Figure S10. Dynamics of Mg^{2+} coordination number with cut-off radius r = 2:8 Å in (a) CC Mg^{2+} simulation with one bound magnesium ion; (b) CC Mg^{2+} simulation with one solvated magnesium ion; and (c) GC Mg^{2+} simulation with one bound magnesium ion.

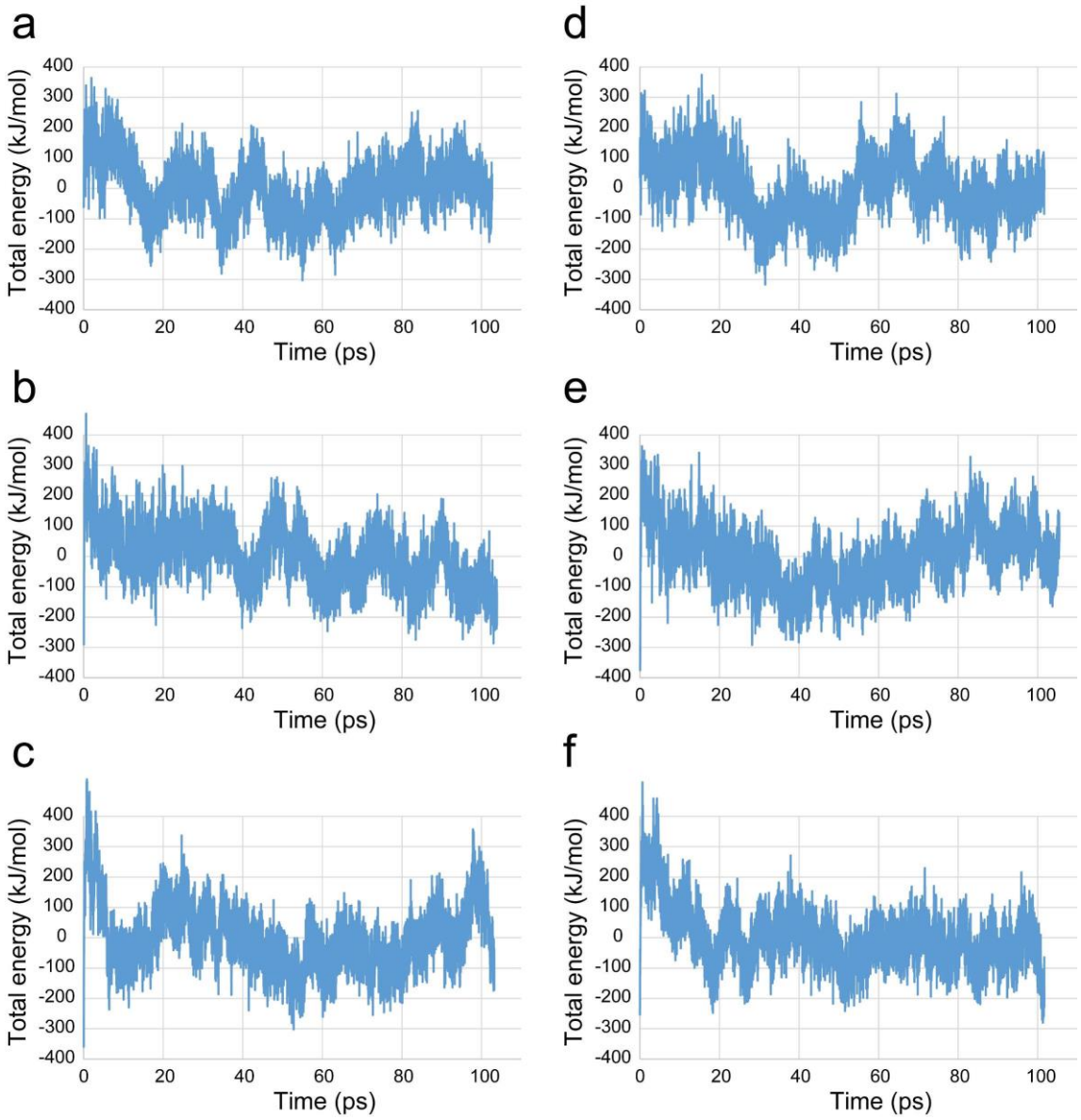

Figure S11. Dynamics of total energy of the system fluctuating around the total energy expectation value 〈E〉 (set to zero in the plots) in (a) CC $2Na^+$ simulation with two bound sodium ions; (b) CC $2Na^+$ simulation with two solvated sodium ions; (c) GC $2Na^+$ simulation with two bound sodium ions; (d) CC Mg^{2+} simulation with one bound magnesium ion; (e) CC Mg^{2+} simulation with one solvated magnesium ion; and (f) GC Mg^{2+} simulation with one bound magnesium ion.