Supporting Information

Structure and Dynamics of Ionic Liquid Tolerant Hyperthermophilic Endoglucanase Cel12A from *Rhodothermus marinus*

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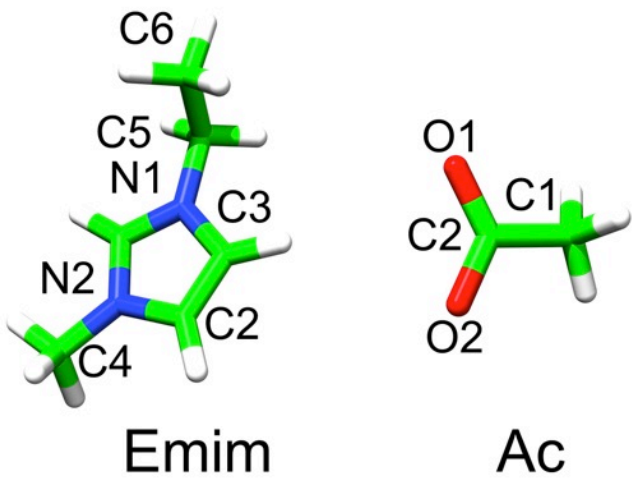

Figure S1. Structure of 1-Ethyl-3-methylimidazolium acetate (EmimAc).

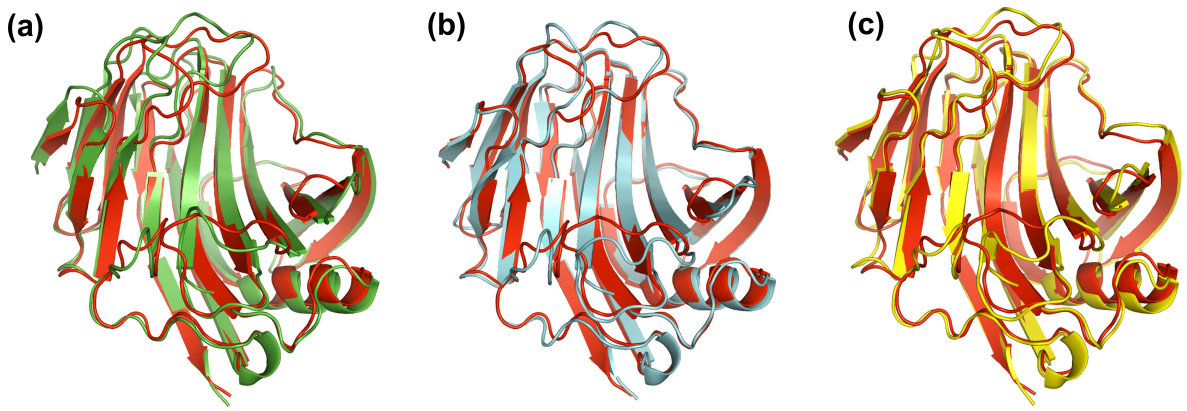

Figure S2. Superpose of the final structure of RmCel12A after 300 ns simulation with the crystal structure shows no significant structural changes of the protein in all the three systems. The crystal structure is colored in red whereas the simulation structures are shown in (a) green (20% EmimAc), (b) cyan (40% EmimAc) and (c) yellow (60% EmimAc) for comparison.

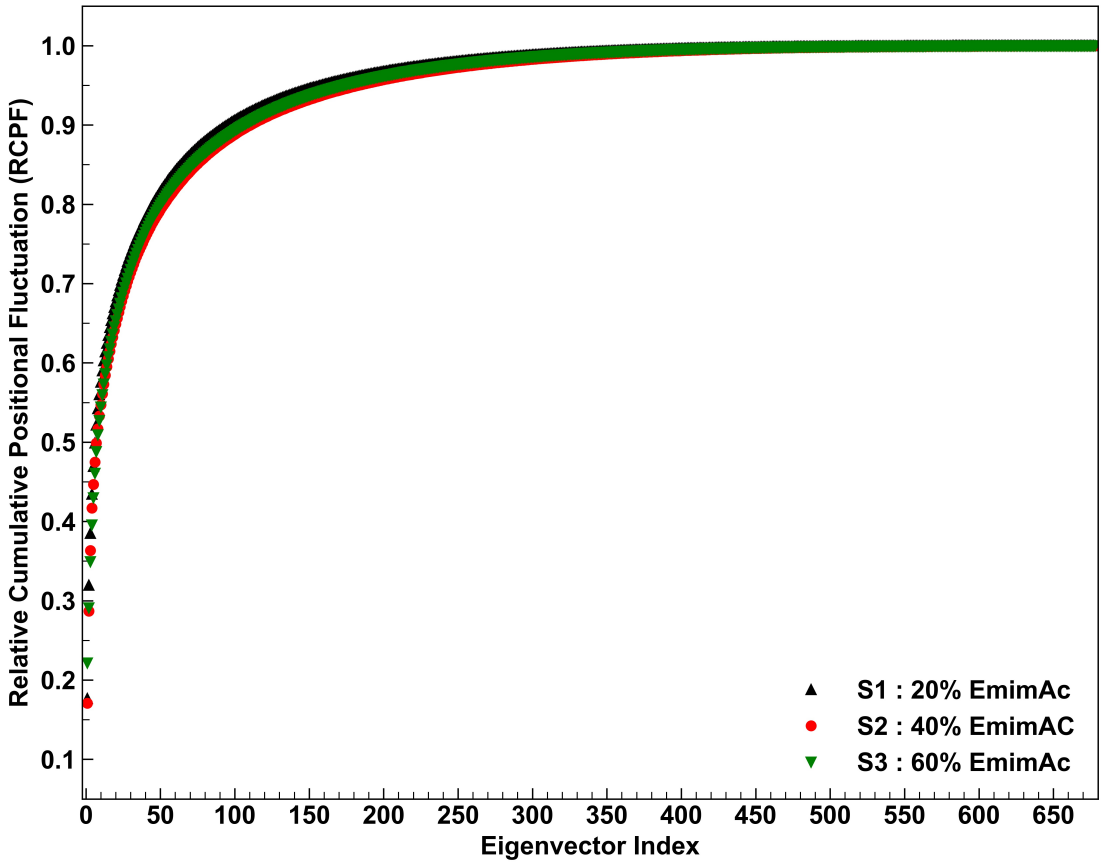

Figure S3. Relative cumulative positional fluctuation (RCPF) of the Eigenvectors for 20% EmimAc (black upper triangle), 40% EmimAc (red circle) and 60% EmimAc (green lower triangle) systems.

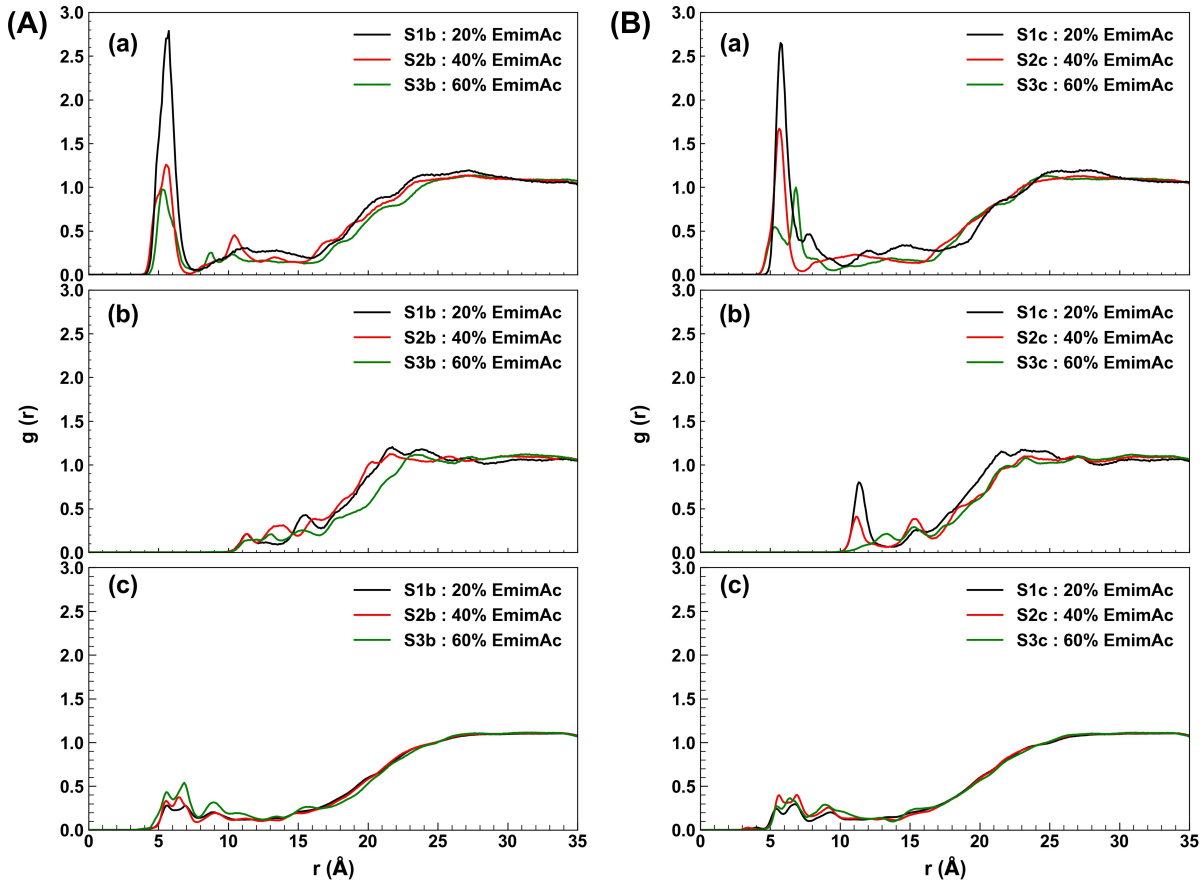

Figure S4. Plot of radial distribution function (RDF) of the solvent molecules with respect to the center of mass (COM) of RmCel12A in 20% EmimAc (black line), 40% EmimAc (red line) and 60% EmimAc (green line) for interactions of (a) RmCel12A-Emim, (b) RmCel12A-Ac, and (c) RmCel12A-water in (A) replicate set b and (B) replicate set c.

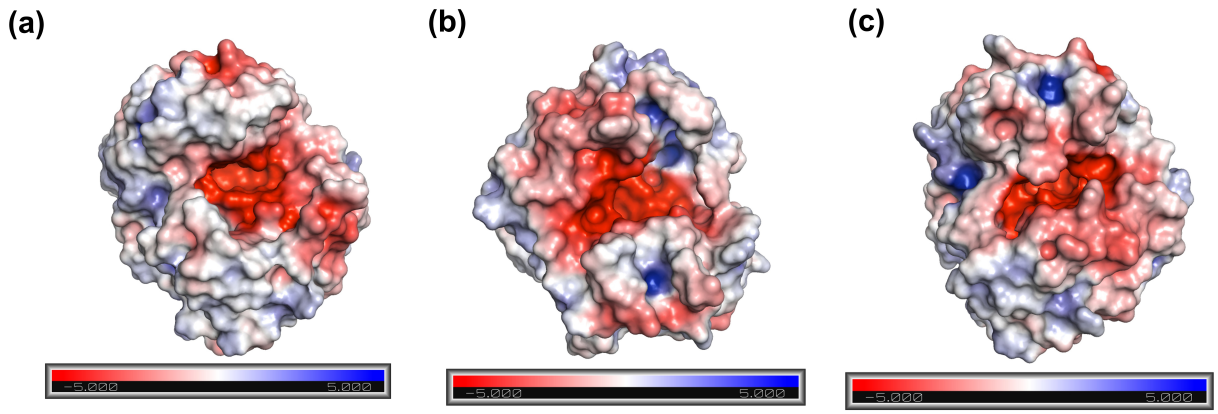

Figure S5. Electrostatic surface charge distribution of the end structures of RmCel12A in (a) 20% EmimAc, (b) 40% EmimAc and (c) 60% EmimAc after 300 ns simulation as obtained from Adaptive Poisson-Boltzmann Solver (APBS) Electrostatics Calculation. Comparatively negative charge distribution can be observed at the active site cleft with respect to the rest of the enzyme surface.

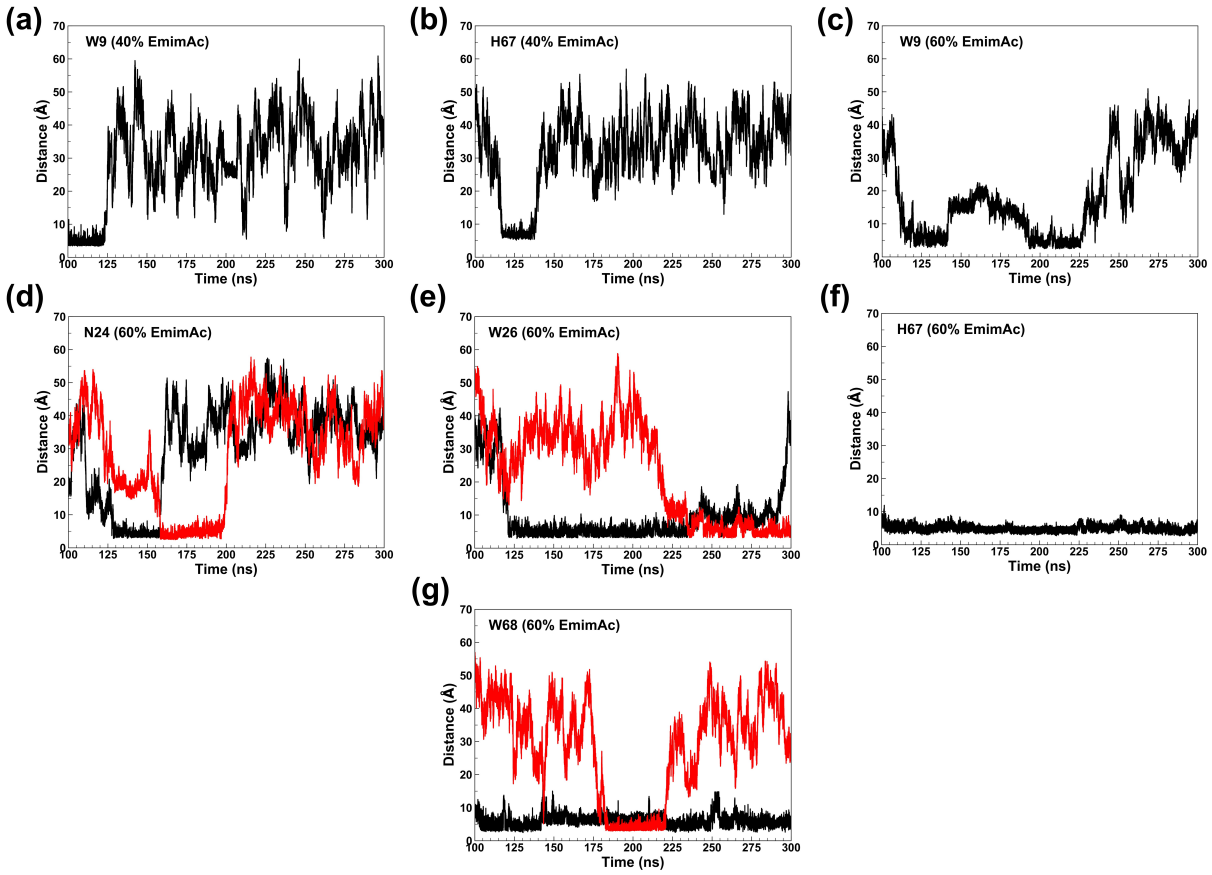

Figure S6. Plot of the time dependent contact distances of the active site residues and the interacting Emim molecules in 40% EmimAc: (a) W9, (b) H67; and 60% EmimAc: (c) W9, (d) N24, (e) W26, (f) H67 and (g) W68. The black and the red color indicate different Emim molecules interacting with a particular amino acid residue.

Table S1. Cumulative fractional occupancy of Emim binding with the catalytic residues of RmCel12A averaged over the three replicate simulations (set a, set b and set c) in 20% EmimAc, 40% EmimAc and 60% EmimAc systems.

Active site Residue	**20% EmimAc**	**40% EmimAc**	**60% EmimAc**
	Average ± Standard Deviation	**Average ± Standard Deviation**	**Average ± Standard Deviation**
W9	-	0.162±0.076	0.179±0.079
N24	-	-	0.212±0.099
W26	-	0.103±0.048	0.225±0.093
H67	-	0.107±0.050	0.236±0.095
W68	-	0.114±0.053	0.217±0.091
R100	-	-	-
E124	-	0.109±0.056	0.310±0.165
W159	-	-	0.345±0.190
W161	-	-	0.605±0.327
Y163	-	-	0.319±0.235
E207	0.519±0.103	0.621±0.176	0.630±0.253
W209	-	-	-