

**Table S3. Sizes of simulated systems.**

System		Number of atoms	Number of counterions (Na <sup>+</sup> )
AMBER	With Ca <sup>2+</sup>	28,951	8
	Without Ca <sup>2+</sup>	31,382	16
CHARMM	With Ca <sup>2+</sup>	31,750	8
	Without Ca <sup>2+</sup>	31,382	16
GROMOS	With Ca <sup>2+</sup>	34,627	8
	Without Ca <sup>2+</sup>	28,559	16
Crystal mimic	With Ca <sup>2+</sup>	586,592	88
Glycosylated	Full glycosylation	88,194	14
	Minimal glycosylation	65,078	8