Table S4. Average Values[a] of the Lattice Parameters of the Core Unit Cell[b] of the MD Crystal Models.

Allomorph	Crystal model	*a* (nm)	*b* (nm)	*c* (nm)	α (deg.)	β (deg.)	γ (deg.)
cellulose Iα	obsd.	0.672	0.596	1.040	118.1	114.8	80.4
		0.677±0.025	0.601±0.020	1.075±0.024	120.1±3.1	112.7±3.0	81.1±2.7
cellulose Iβ	obsd.	0.778	0.820	1.038	90.0	90.0	96.5
		0.762±0.021	0.825±0.019	1.077±0.018	90.5±1.8	90.3±2.1	97.6±2.4
cellulose II	obsd.	0.810	0.903	1.031	90.0	90.0	117.1
	A36	0.840±0.023	0.883±0.021	1.074±0.018	90.5±2.0	89.7±2.0	118.0±2.6
	B36-1	0.849±0.022	0.879±0.021	1.072±0.018	89.8±2.0	90.1±2.0	118.2±2.6
	B36-2	0.847±0.023	0.878±0.021	1.074±0.018	89.6±1.9	89.8±2.0	118.4±2.7
cellulose III_I	obsd.	0.445	0.785	1.031	90.0	90.0	105.1
	A48	0.446±0.016	0.754±0.025	1.074±0.018	90.0±1.9	89.9±2.2	93.6±3.3
	B48	0.446±0.018	0.755±0.027	1.074±0.023	90.1±2.3	89.9±2.6	93.4±3.5

[a] The values were averaged form the final 5 ns trajectories.

[b] The innermost unit cell in the crystal model.