Table S1 Enthalpy of solvation of glycine aqueous solution as bulk with different ethanol concentration

Ethanol mole fraction [-]	Enthalpy of solvation [kJ mol^{-1}]
0.0052	-121.45
0.0213	-118.99
0.0294	-118.37
0.0466	-116.86
0.0773	-115.27
0.1154	-115.10
0.2268	-115.77

Table S2 List of hydrogen bond (N-H…O_g) of glycine alpha and gamma polymorph

polymorph	Distance H…O_g [A]	Distance N…O_g [A]	Angle of N-H…O_g [degree]
Alpha	2.413	2.953	115.74
	2.186	3.080	156.29
	1.794	2.778	167.51
	1.888	2.854	168.7
Gamma	1.941	2.807	159.89
	1.934	2.802	163.29
	2.121	2.983	173.5

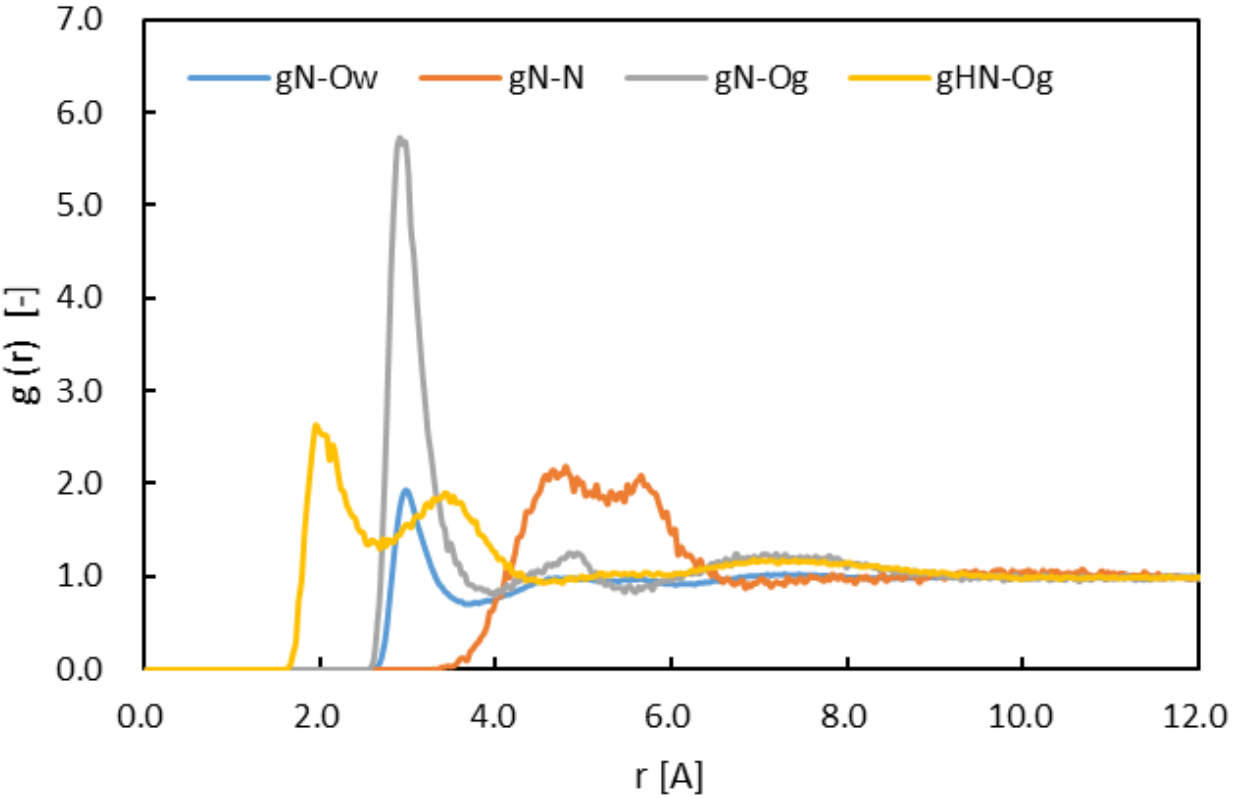


Fig. S1 Radial distribution function, g(r) of N-O_w (oxygen of water), N−N, N−O_g (oxygen of glycine) and HN-O_g (hydrogen bonded to N) of glycine zwitterion aqueous solution of at C = 3.33 mol kg^{-1}.

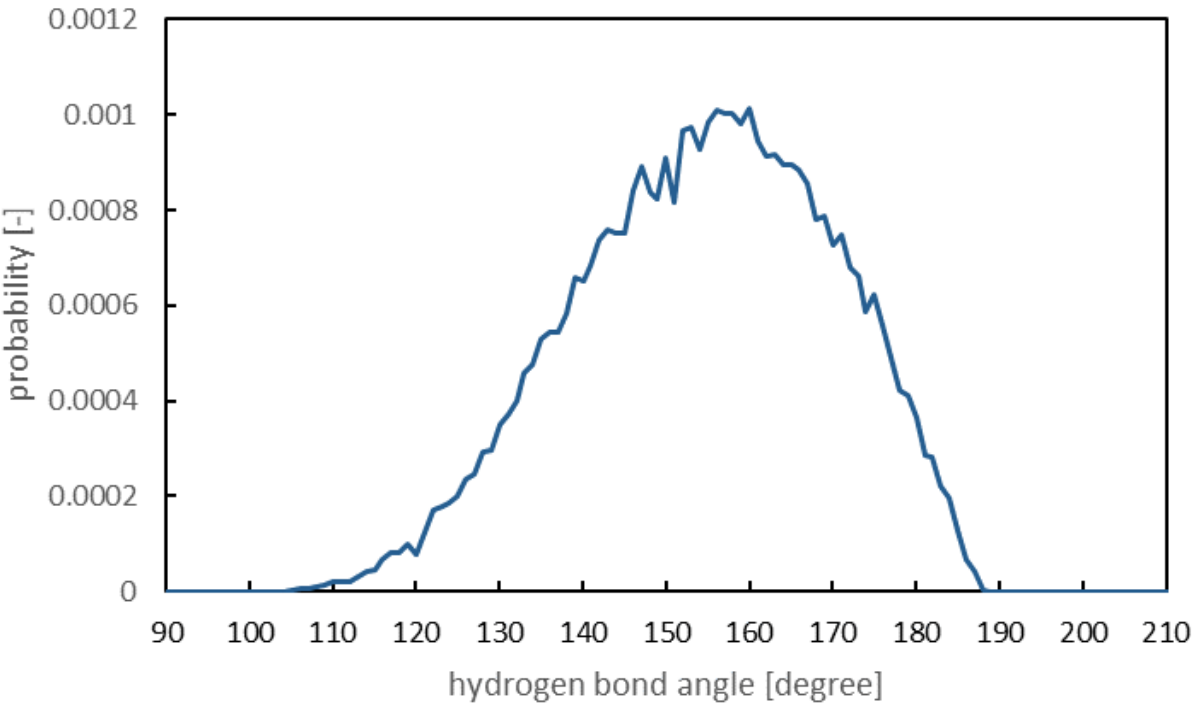


Fig. S2 Angle spectra of hydrogen bond (HN-N…O_g) of glycine-glycine cluster in C = 3.33 mol kg^{-1} glycine aqueous solution as bulk

a)

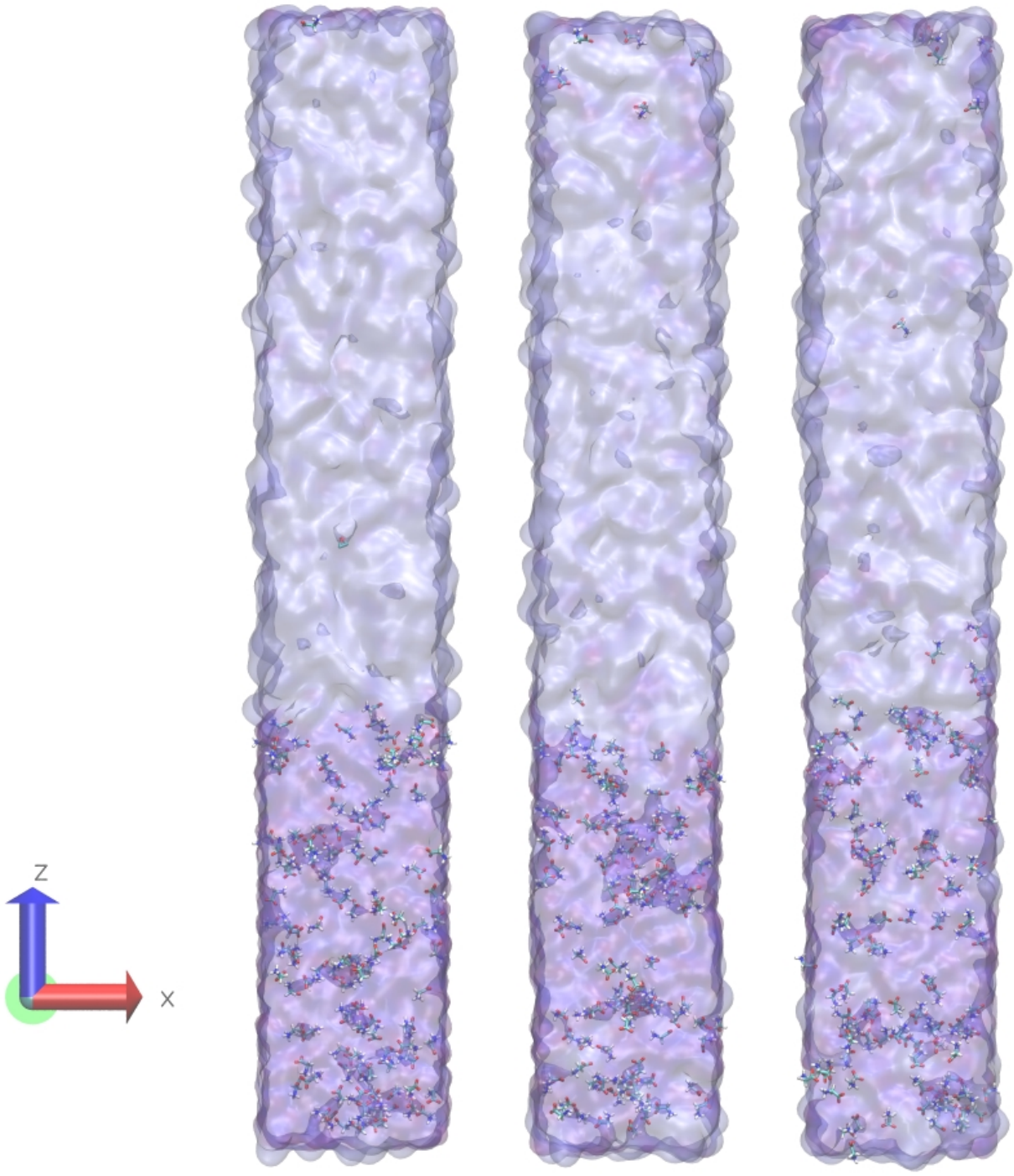


Fig. S3 Snapshots of glycine aqueous solution and ethanol system at t = 0.0, 2.5 and 5.0 ns at C = 2.94 mol kg^{-1}.

c)

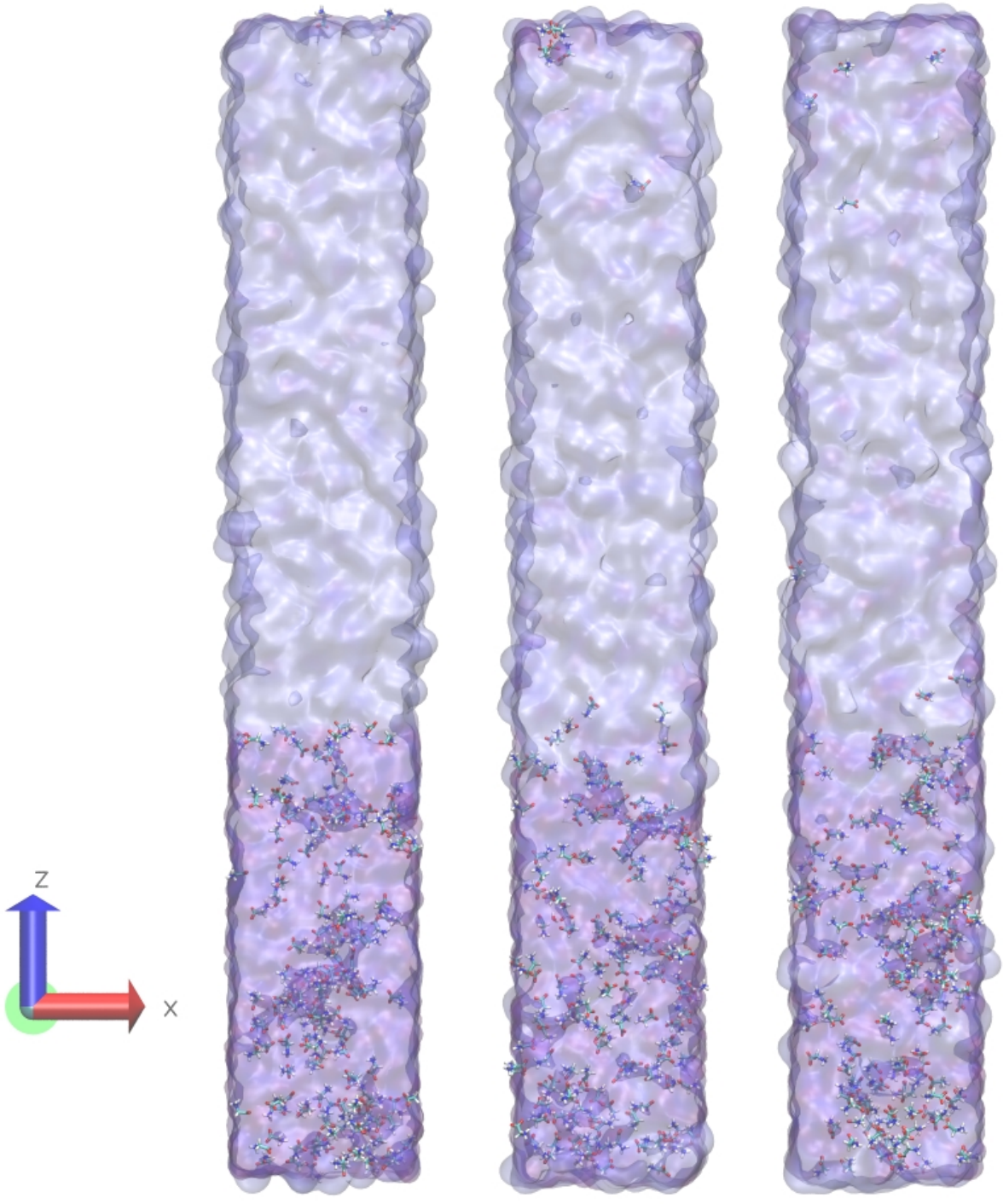


Fig. S4 Snapshots of glycine aqueous solution and ethanol system at t = 0.0, 2.5 and 5.0 ns at C = 3.72 mol kg^{-1}.

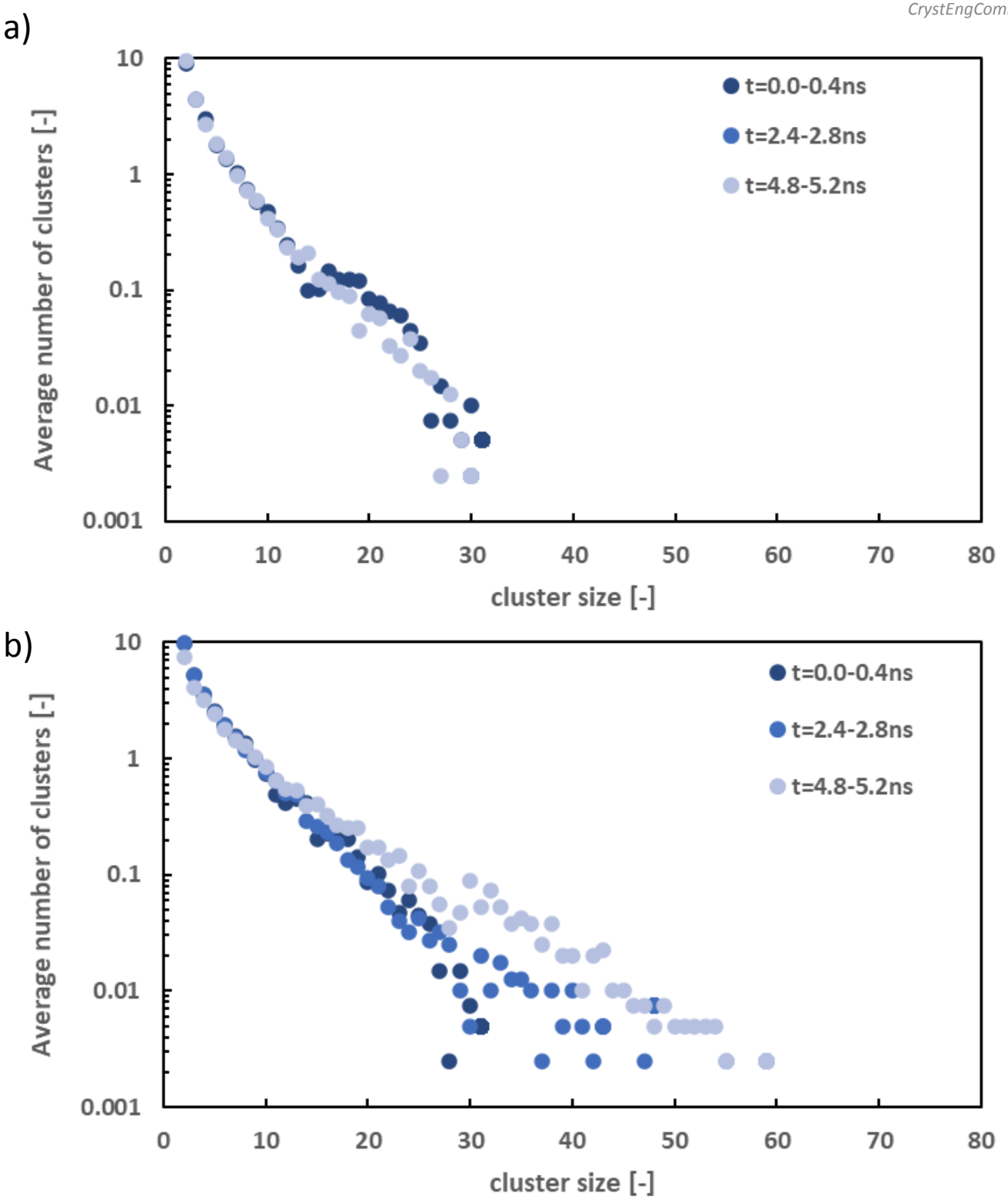
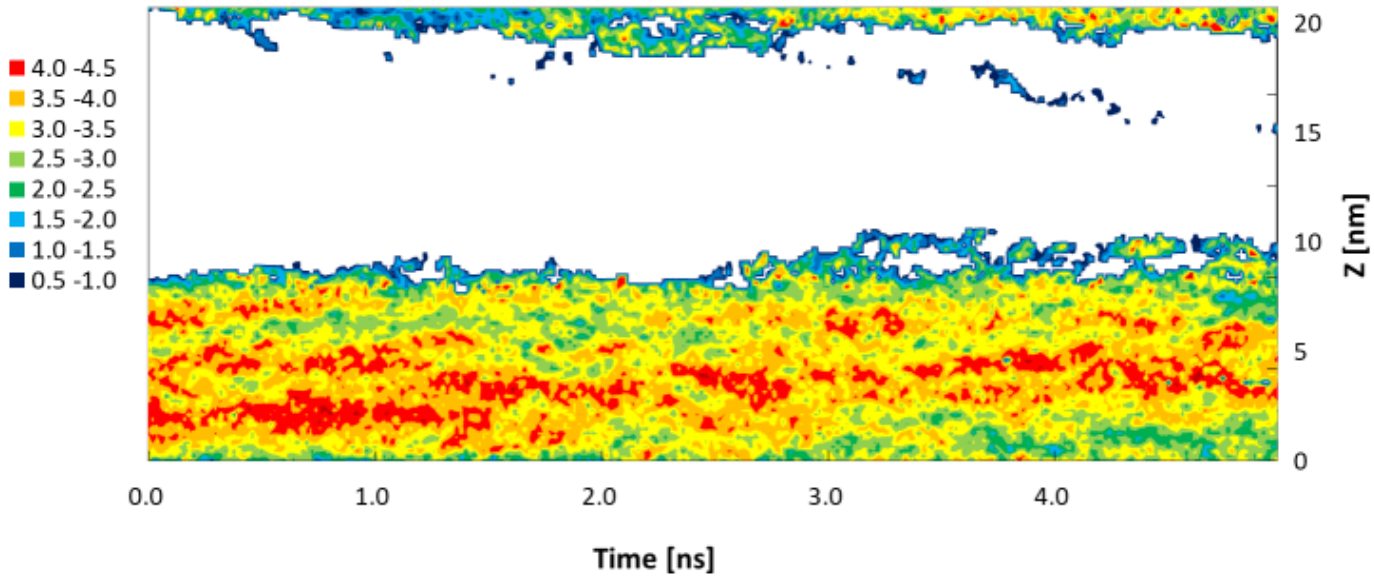


Fig. S5 clustering behavior of the system: semilog histograms of the average number observed versus cluster size at a) C = 2.94 mol kg^{-1} and b) C = 3.72 mol kg^{-1}.

a)



c)

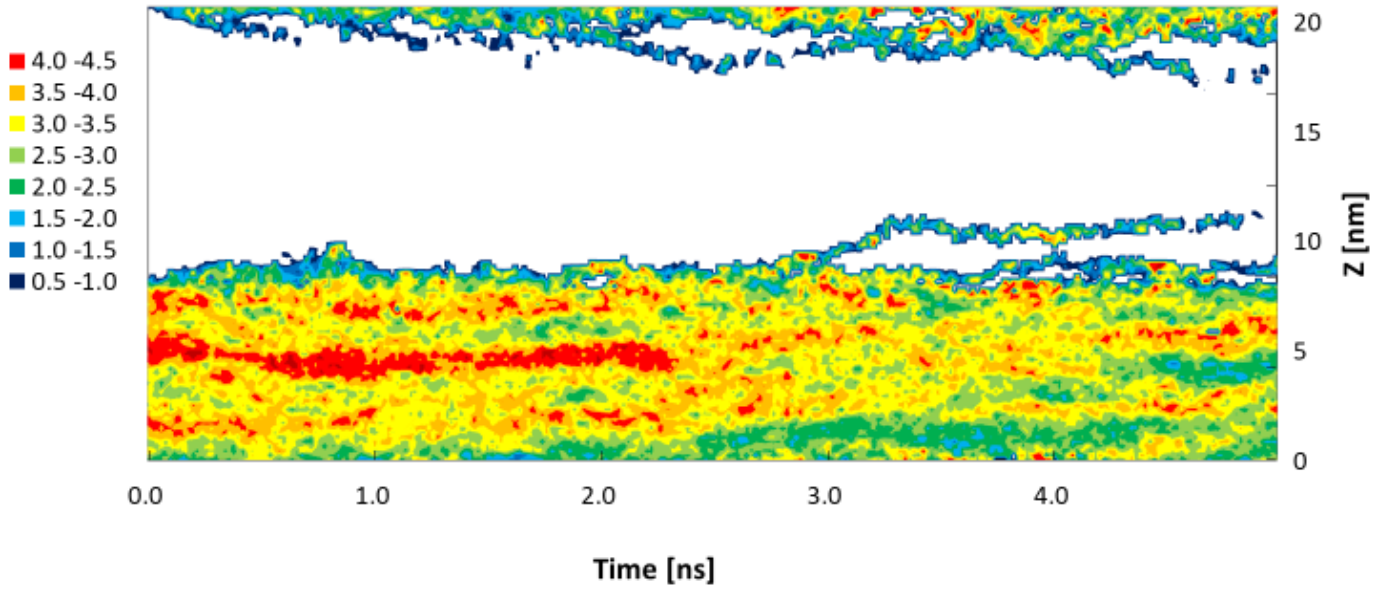
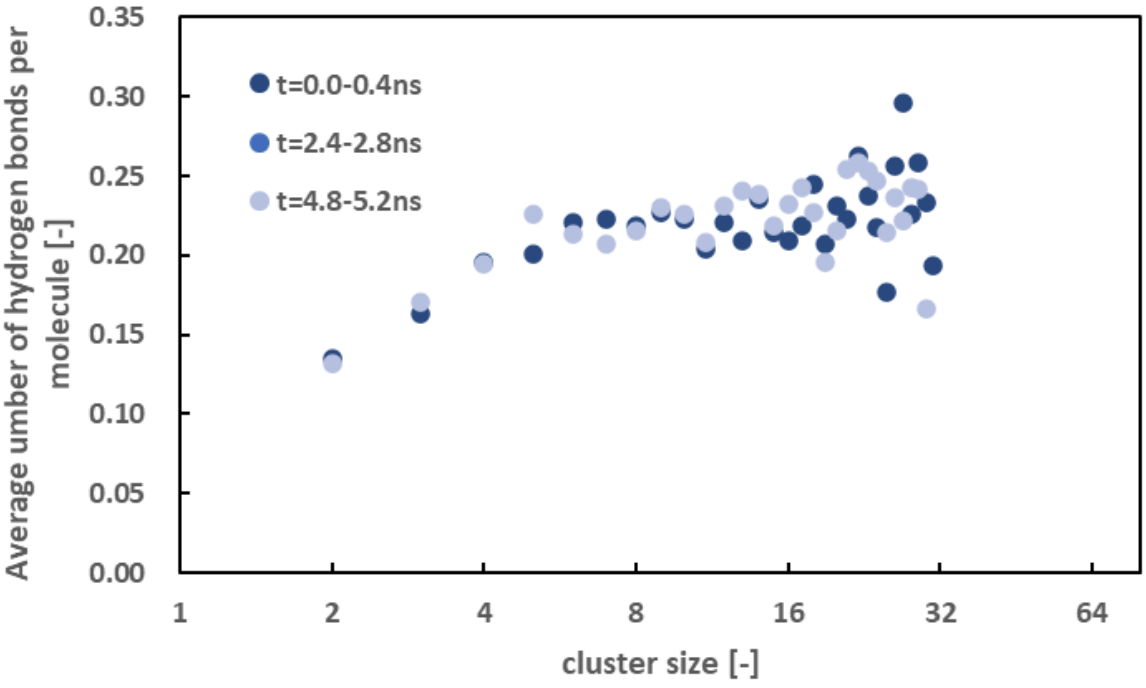


Fig. S6 Coordination number of N-O_w vs. time (t = 0.0-5.0 ns) at a) C = 2.94 and b) C = 3.72 mol kg^{-1} of glycine aqueous solution.

a)



b)

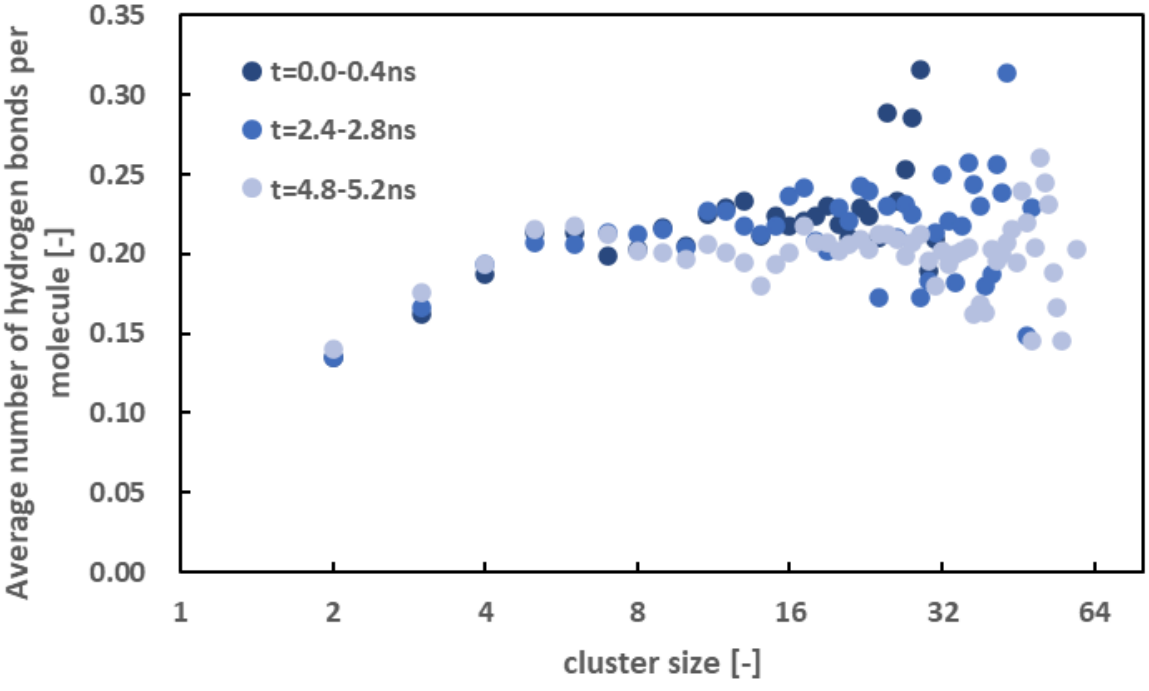


Fig. S7 Average number of hydrogen bonds per molecule vs. cluster size at a) C = 2.94, b) C = 3.72 mol kg^{-1} of glycine aqueous solution.