Supplementary Table 1: Density of the systems 0% glycerol, 40% glycerol and 100% glycerol after 100 ns of MD production and its comparison with theoretical [1] and experimental data [2].

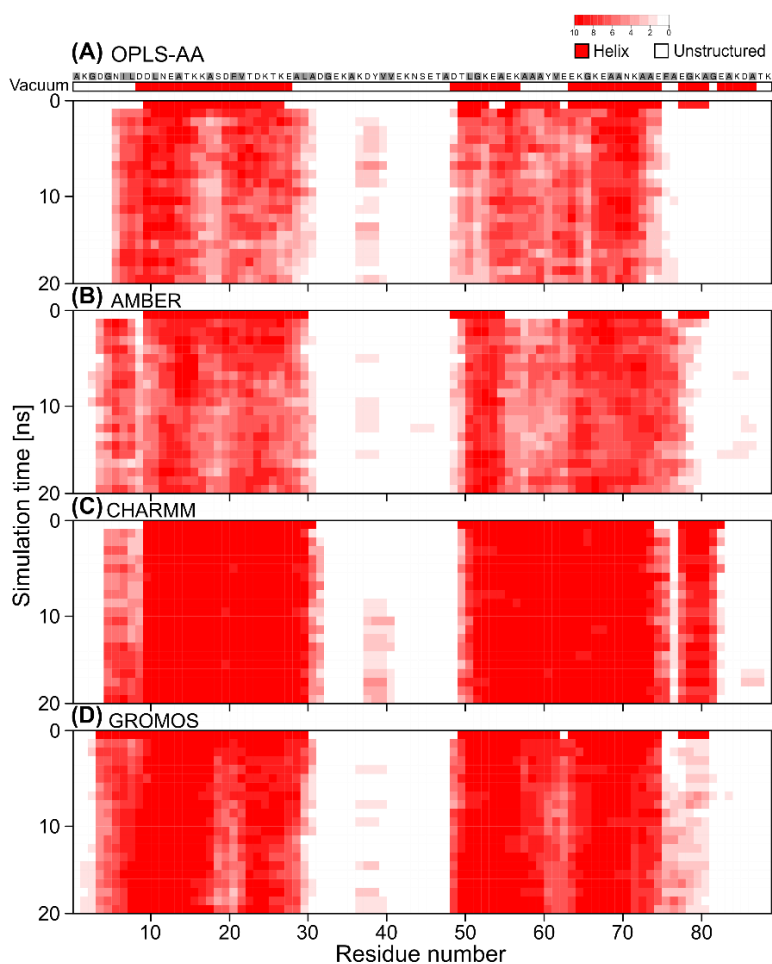|	Calculate (kg/m^3)	Theoretical (kg/m^3)	Experimental (kg/m^3)
100% water	997.85 ± 0.01	995	997
40% glycerol	1087.85 ± 11.30	1103	1106
100% glycerol	1214.19 ± 7.59	1223	1261

Fig. S1: Changes in the secondary structure content of the COR15A homology model during 20 ns of MD simulation in single-residue resolution using four different force fields. Amino acids in α- helical conformation are shown in red, those in a random coil formation in white. The colour intensity reflects the convergence of helix formation of a specific residue across 10 MD simulations replicates. Hydrophobic residues are labelled in grey.
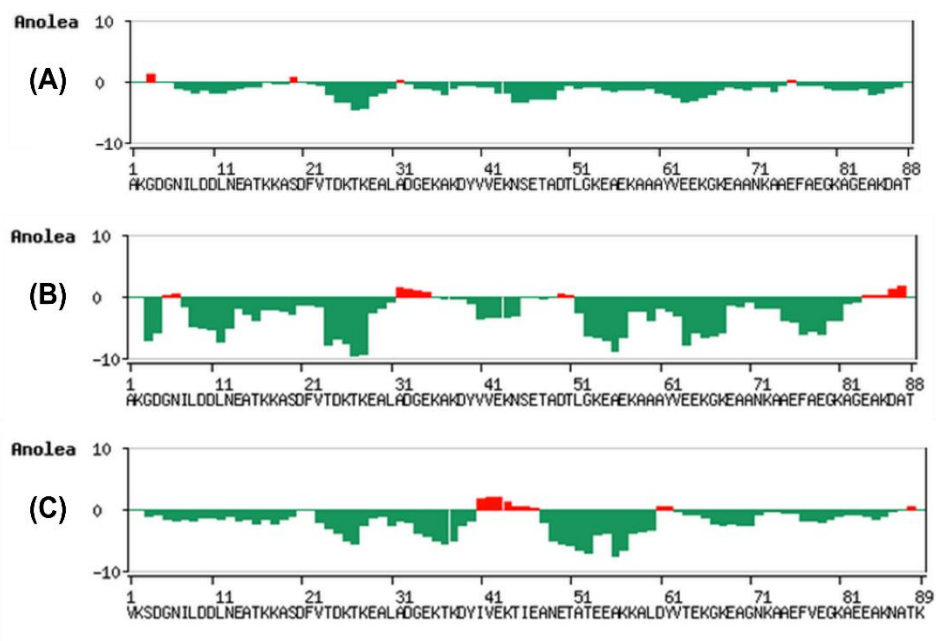
Fig. S2: Evaluation of non-local environment interactions performed by the atomic empirical mean force potential ANOLEA on each heavy atom in COR15A_TH (A), COR15A (B) and COR15B (C) models. Negative energies (green) represent favorable interactions of the respective residue.
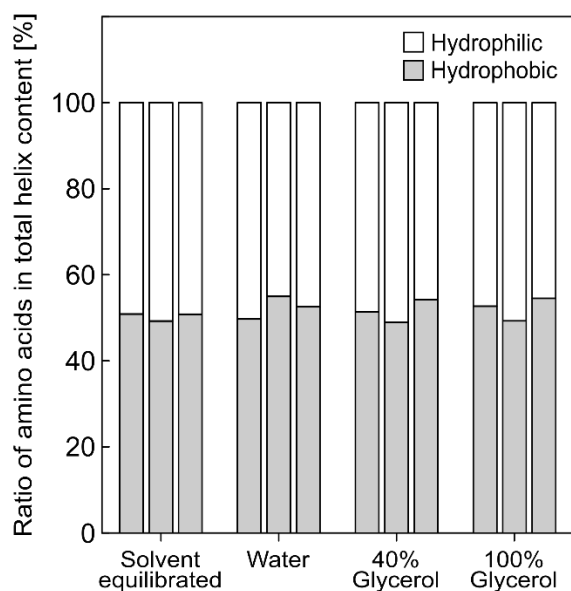

Fig. S3: Contribution of hydrophobic and hydrophilic amino acids to total amount of amino acids in an α-helical conformation in the beginning (after solvent equilibration) and after 30 ns of MD simulation in all three solvent systems. Groups of bars represent the three models in the order COR15A_TH, COR15A, COR15B, respectively.
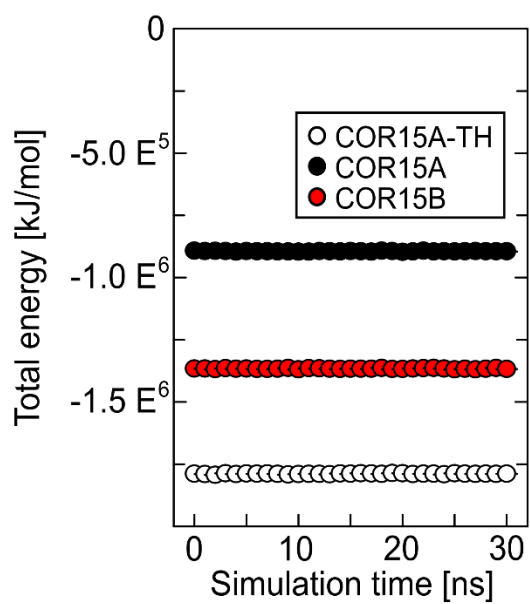
Fig. S4: Analysis of potential energy during 30 ns MD simulations of COR15A_TH (white), COR15A (black) and COR15B (red)
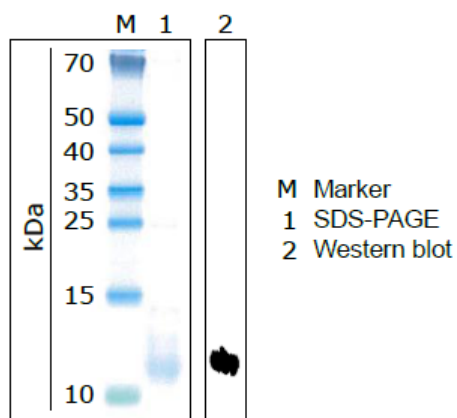

Fig. S5: SDS-PAGE and Western blot analysis of recombinant untagged COR15A. The membrane was probed with antiCOR15A antibody. The protein ladder on the left hand side indicates molecular masses of standard proteins.
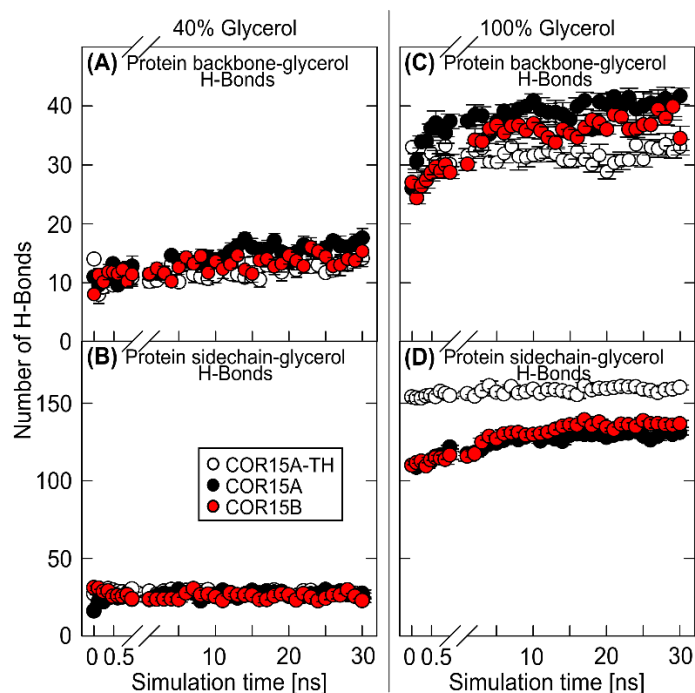
Fig. S6: Contributions of intermolecular protein backbone-glycerol (A, C) and sidechain-glycerol (B, D) H-bonds during 30 ns MD simulations of COR15A_TH (white), COR15A (black) and COR15B (red) in the presence of 40% (A, B) and 100% (C, D) glycerol.
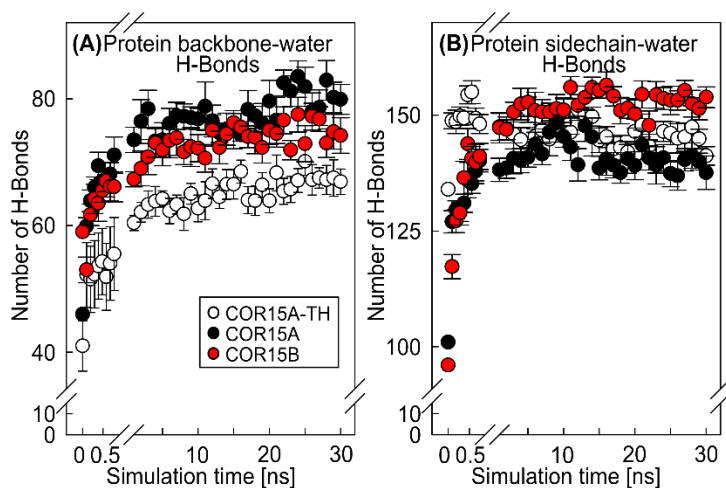

Fig. S7: Contributions of intermolecular protein backbone-water (A) and sidechain-water (B) H-bonds during 30 ns MD simulations of COR15A_TH (white), COR15A (black) and COR15B (red) in water.
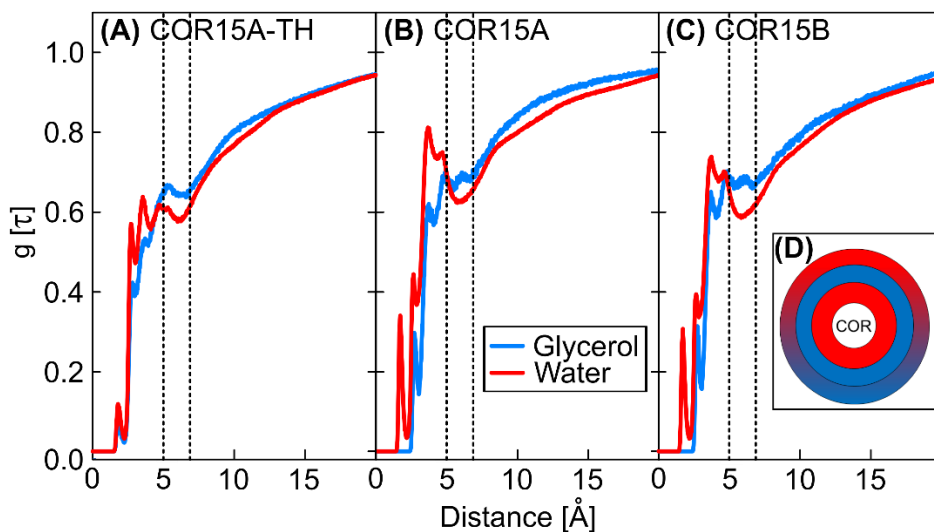
Fig. S8: Radial distribution function (RDF) analysis of water (red) and glycerol (blue) molecules around COR15A_TH (A), COR15A (B) and COR15B (C) during 30 ns MD simulations in 40% glycerol. A schematic drawing of interactions between COR15 proteins and solvents is shown in panel (D).

References:

1   A. V. Egorov, A. P. Lyubartsev and A. Laaksonen, *J. Phys. Chem. B*, 2011, **115**, 14572.

2   D. R. Lide, *CRC handbook of chemistry and physics*, Taylor & Francis, 85th edn, 2004.