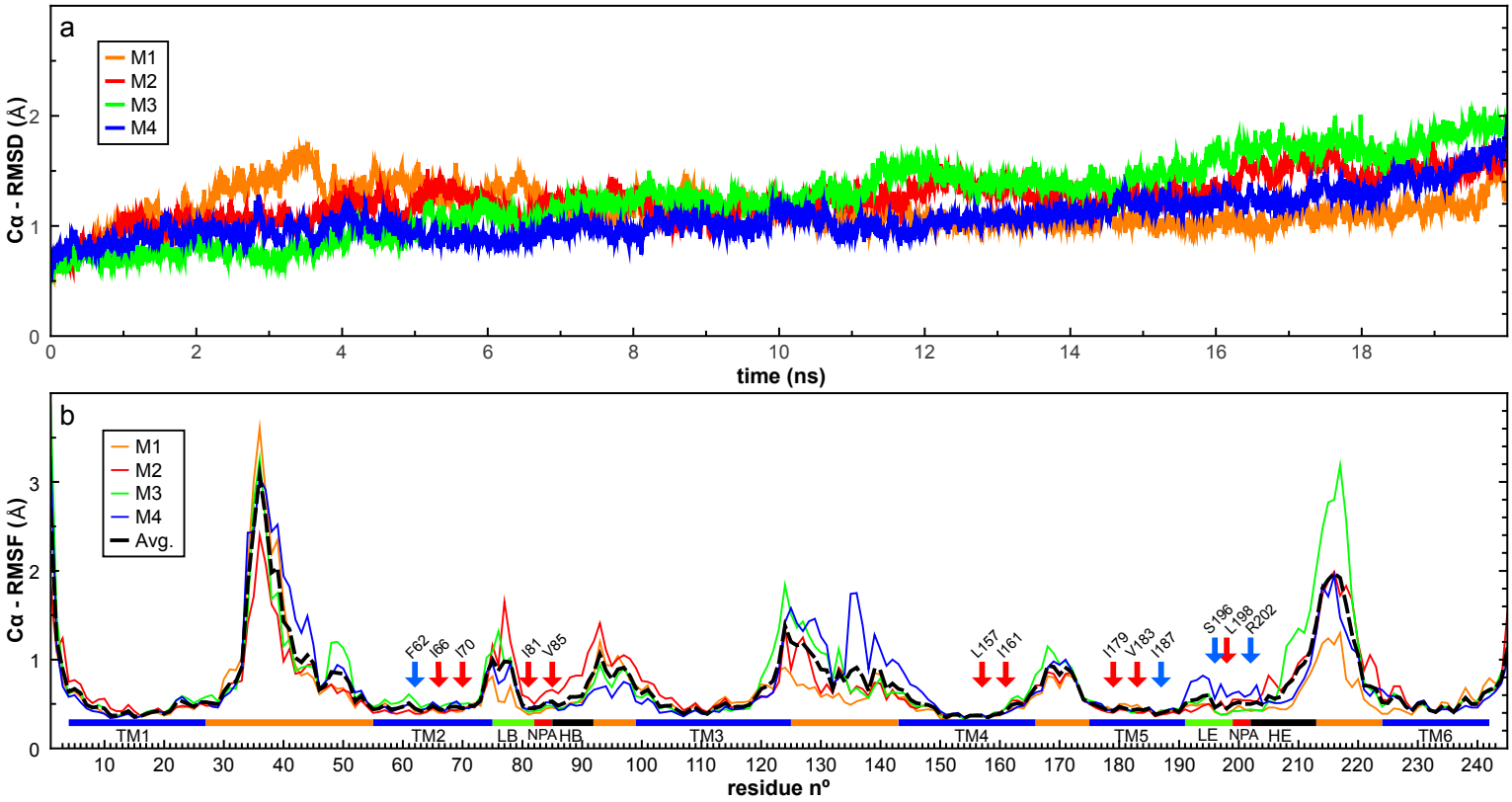

Fig S1. Cα-RMSD and Cα-RMSF of the simulated AqpM tetramer.
(a) Time evolution of Cα-RMSD for each AqpM monomer obtained from the 20ns production run. The last conformation obtained from the minimization-relaxation procedure (see methods) was used as reference structure for the measurement. (b) Cα-RMSF for each AqpM monomer obtained from the 20ns production run. Each coloured solid line represents a monomer. The dashed black line represents the average RMSF. The solid lines below the curves indicate secondary structure elements of AqpM (blue = TM-helix; orange = loops; green = loops B and E; red = NPA motifs; black = helix B and E). Light blue arrows indicate residues that comprise the selectivity filter (S.F) of AqpM; red arrows indicate hydrophobic residues that line the AqpM pore.