SUPPLEMENTARY MATERIAL

Figure S1. Time evolution of the backbone heavy atom RMSD from the initial structure in the: a) Cpep+ simulations, b) Cpep0 simulations, c) Mut+ simulations, d) Mut0 simulations. Black: Simulations in water at 277 K, Red: Simulations in water at 300 K, Green: Simulations in 8M urea.

Figure S2. C_α pair-wise RMSD matrix plots. a) Cpep+ simulation in water at 277 K, a') Cpep+ simulation in water at 300 K, a") Cpep+ simulation 8M urea, b) Cpep0 simulation in water at 300 K, b') Cpep0 simulation 8M urea, c) Mut+ simulation in water at 277 K, c') Mut+ simulation in water at 300 K, c") Mut+ simulation 8M urea, d) Mut0 simulation in water at 300 K, d') Mut0 simulation 8M urea. The color reflects the C_α RMSD in Ångstroms according to the scale shown.

Figure S3. Distributions of the number of hydrogen bonds that the peptide accepts from water with 1.8 Å (open symbols) and 2.4 Å (solid symbols) cutoffs. Black is used for simulations in water at 277 K, red for water at 300 K and green for 8M urea simulations

Figure S1

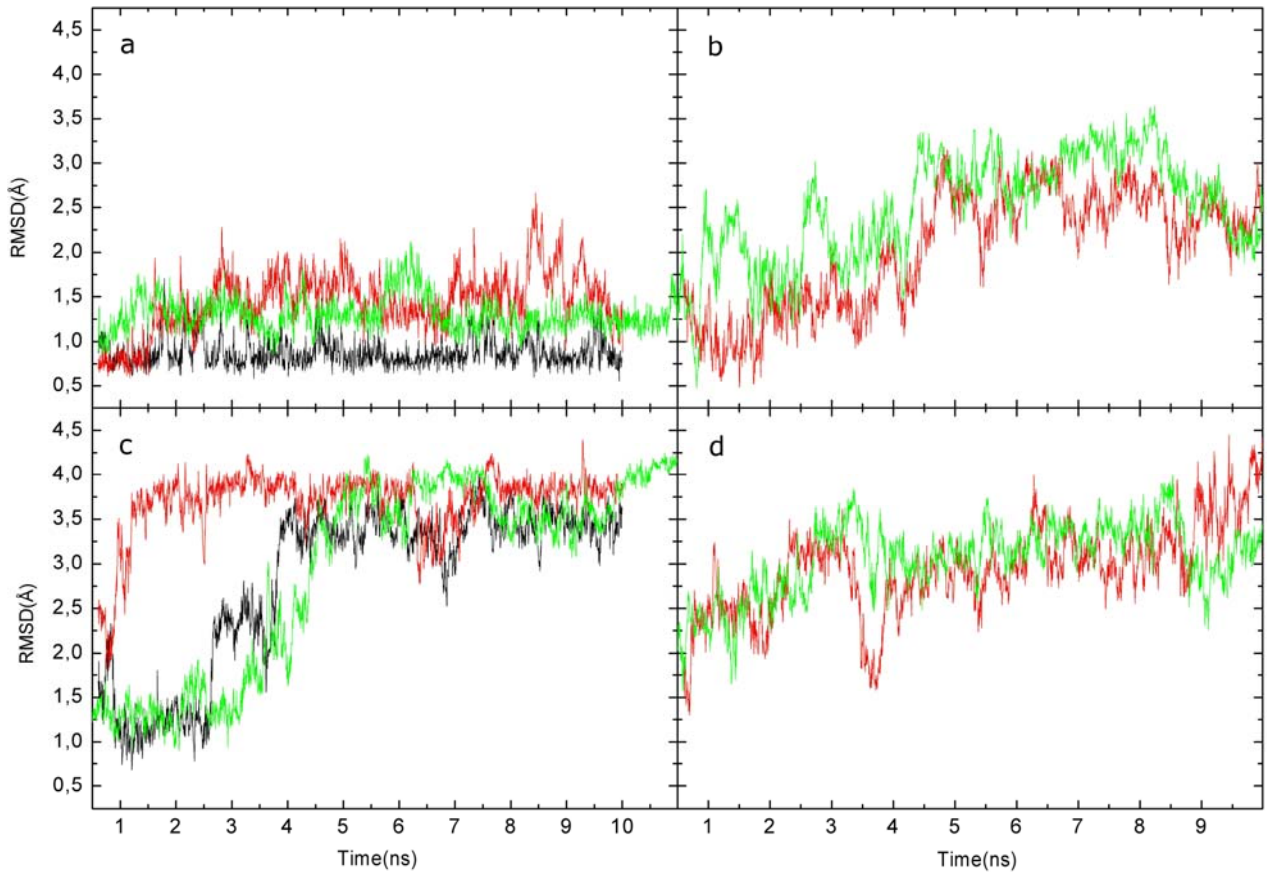

Figure S2

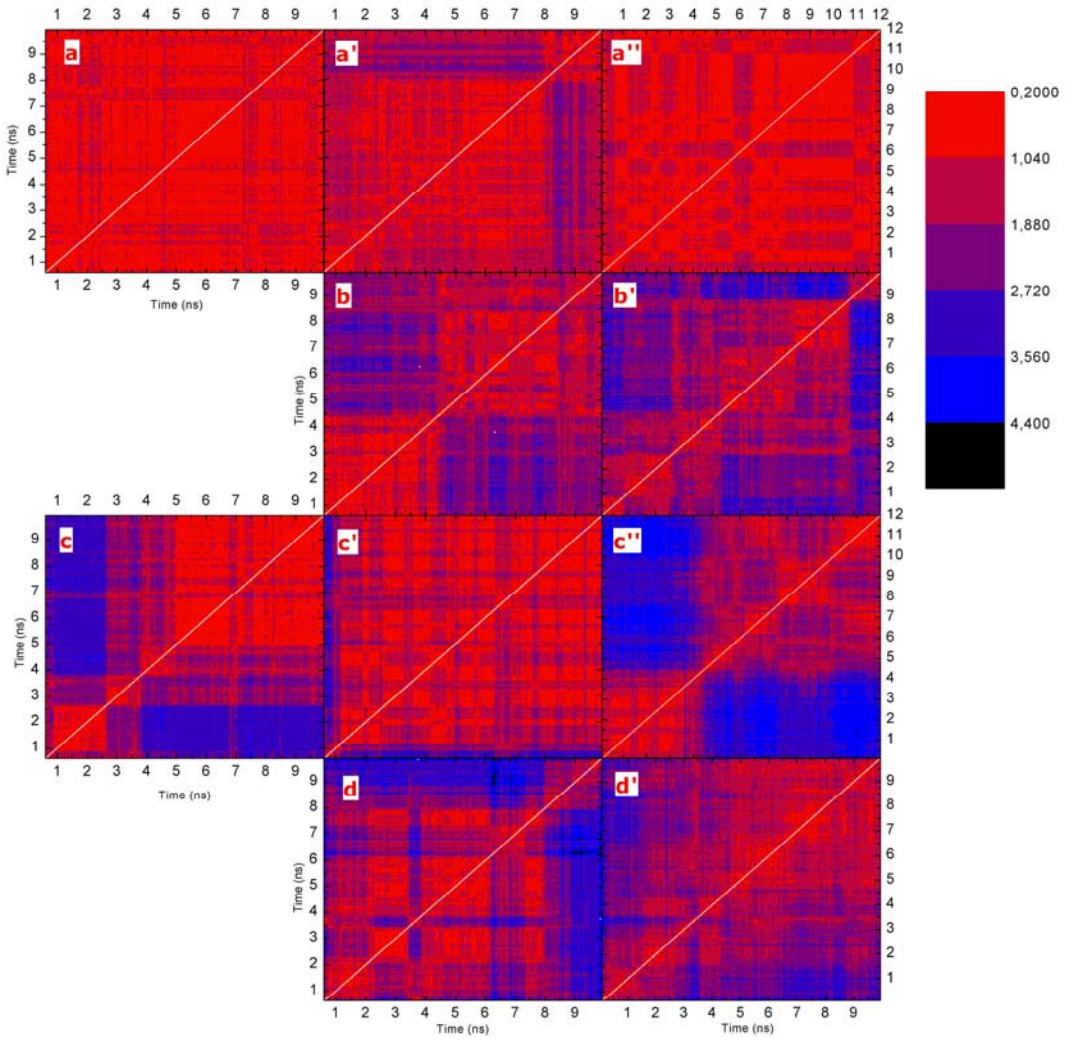

Figure S3

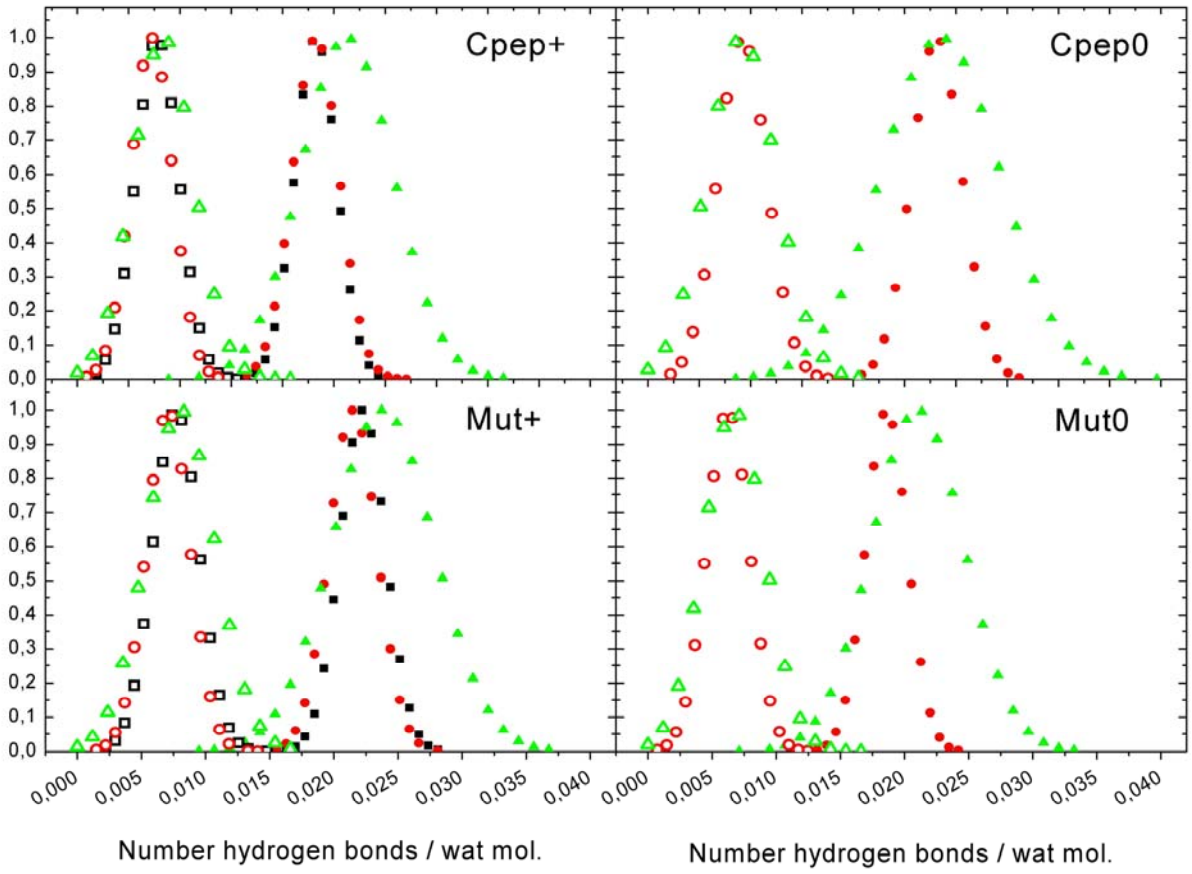
Cpep+
Cpep0
Mut+
Mut0
1,0
0,9
0,8
0,7
0,6
0,5
0,4
0,3
0,2
0,1
0,0
0,000
0,005
0,010
0,015
0,020
0,025
0,030
0,035
0,040
Number hydrogen bonds / wat mol.
Number hydrogen bonds / wat mol.

Table S1 Standard deviations (SD) for the normal distributions of the peptide oxygen-water hydrogen distribution with 2.4 Å and 1.8 cutoff

	$SD_{2.4Å}$	$SD_{1.8Å}$
Cpep+ 277 K	0.0016	0.0017
Cpep+ 300 K	0.0018	0.0016
Cpep+ 8M	0.0036	0.0024
Cpep0 300 K	0.0020	0.0019
Cpep0 8M	0.0046	0.0027
Mut+ 277 K	0.0018	0.0018
Mut+ 300 K	0.0019	0.0017
Mut+ 8M	0.0040	0.0027
Mut0 300 K	0.0021	0.0019
Mut0 8M	0.0045	0.0029