Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Comparison of a IBI and FM potential:

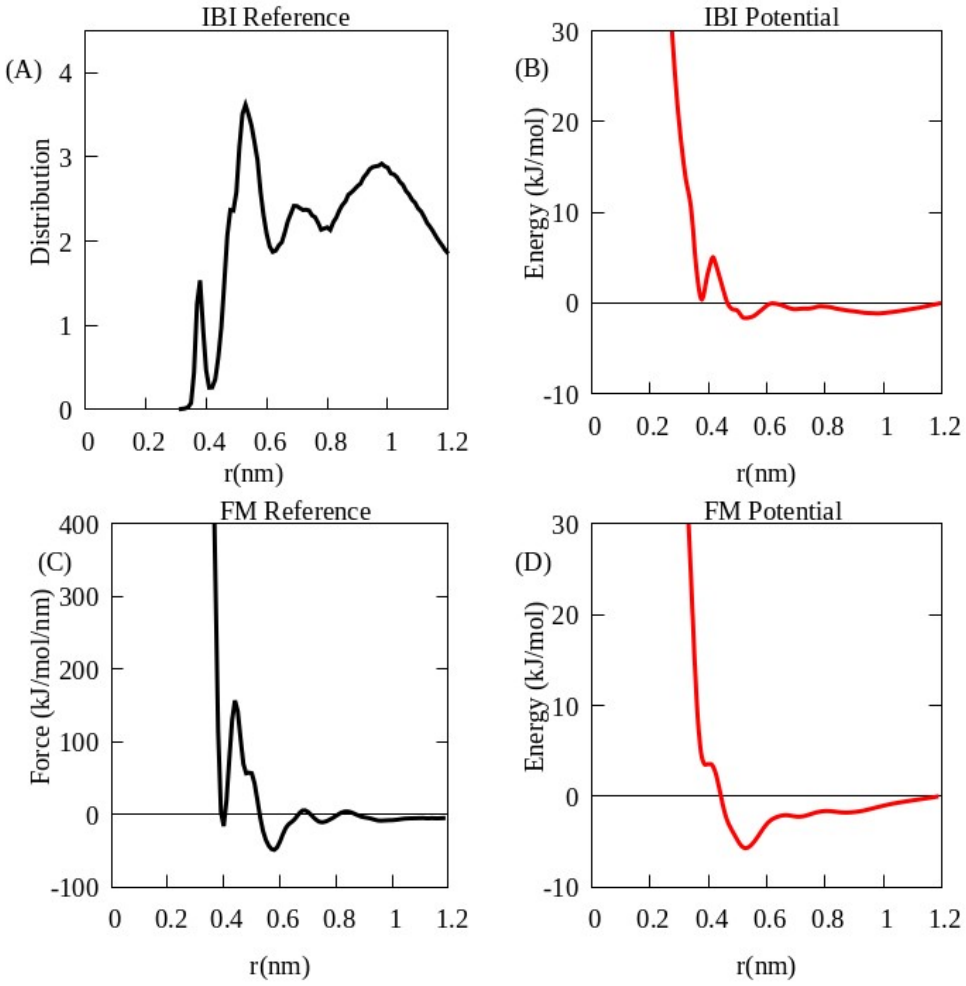


Fig. SI.1: (A) shows the reference RDF for the IBI potential. (B) shows the IBI potential. Similarly, (C) shows the reference forces for the FM potential. (D) shows the FM potential. The potentials are generated with the 25 AA V_2K peptide system as a reference.

Water-water RDF in a single peptide system:

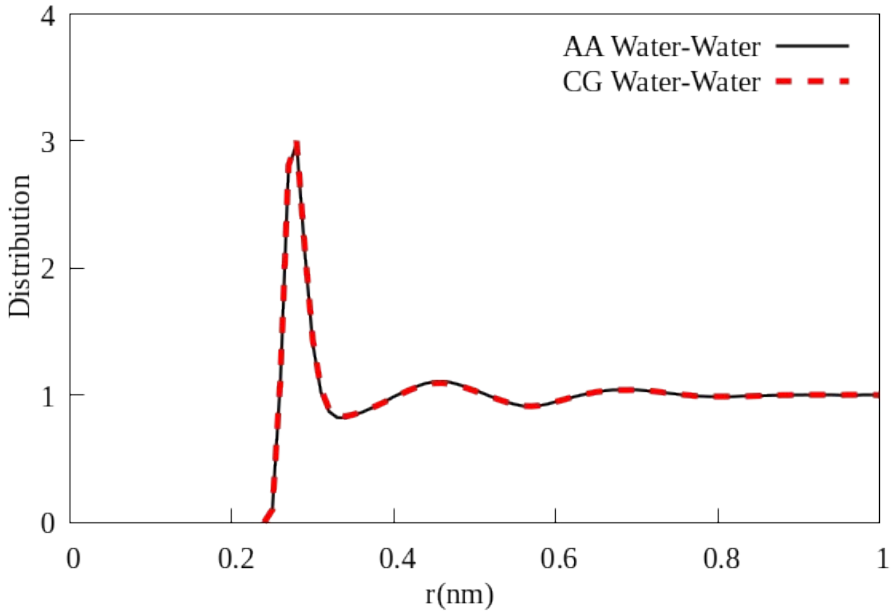


Fig. SI.2: Water-water radial distribution function in a system with a single V_6K_2 peptide. Color scheme: AA (black) and CG (red) systems.

Water-water RDFs in Multiple Peptide Systems:

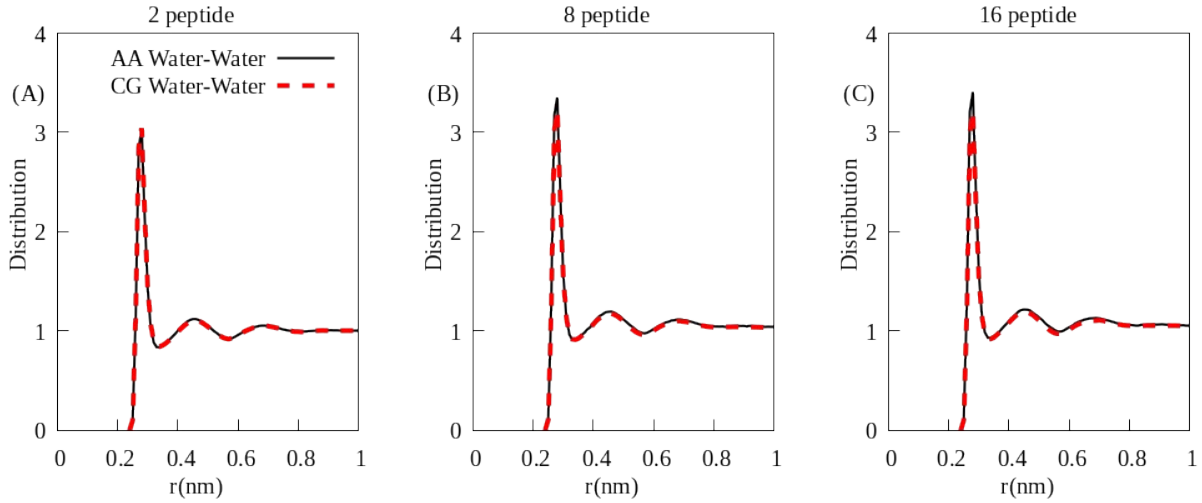


Figure SI.3: AA and CG water-water radial distribution functions are compared for 2,8 and 16 peptide systems.

Water-water RDFs in 128 peptide systems:

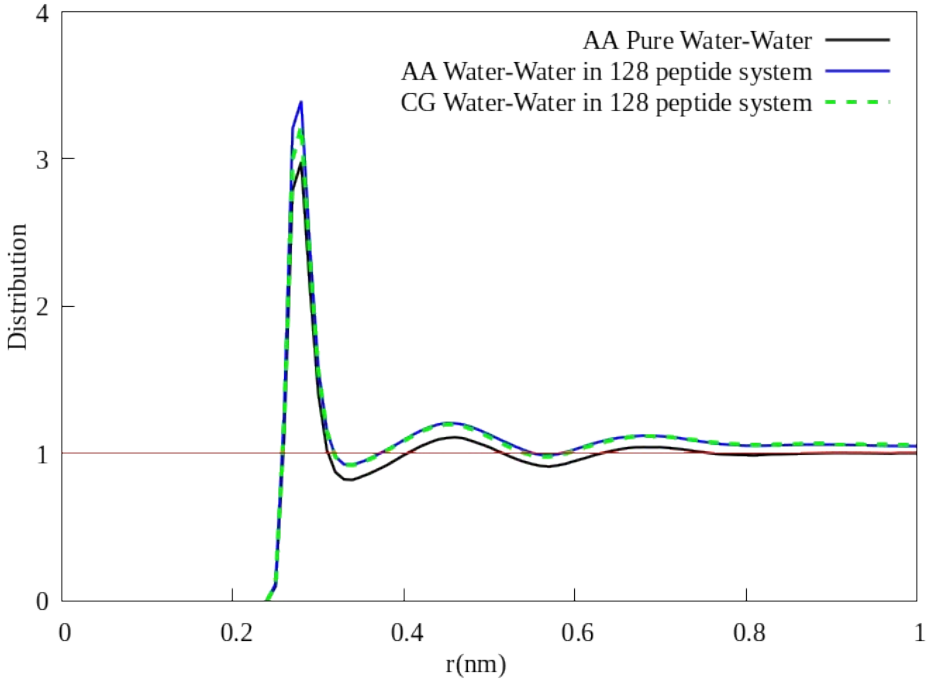


Figure SI.4: Water-water radial distribution functions are compared for pure water system, 128 AA peptides in water and 128 CG peptides in water.

Transferability of peptide-water potentials from V_2K to V_6K_2:

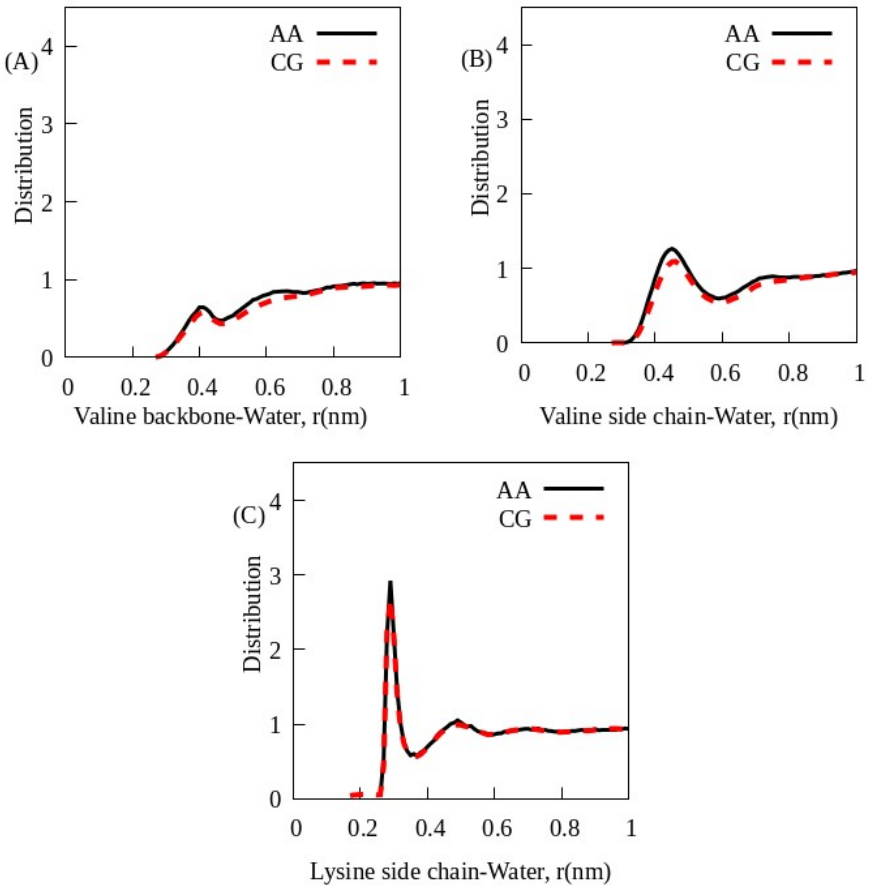


Fig. SI.5. Peptide-water radial distribution functions for the CG V_6K_2 peptide system. The peptide-water potentials developed with the V_2K peptide is used to model this system.

Figure SI.5 shows that the peptide-water potentials developed for the CG V_2K peptide are transferable to the CG V_6K_2 peptide. The solvation structure of the CG V_6K_2 peptide is in good agreement with the corresponding reference. There is an extremely minor disagreement between the RDFs at ~ 0.45 nm in the Valine side chain-water interaction (Figure SI.5.B) and at ~ 0.3 nm in the Lysine side chain-water interaction (Figure SI.5.C).

Ions coordinated with Lysine residues:

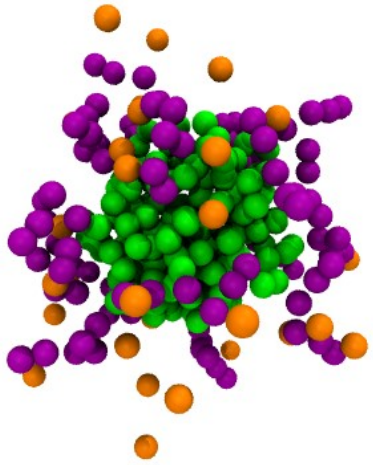


Figure SI.6: Micelle formed by self-assembly of 16 V_6K_2 peptides (CG representation) in aqueous solution. Ions (orange) are well-coordinated with the Lysine (purple) residues. The green color beads are the Valine residues.

Stepwise increase in peptide chain length:

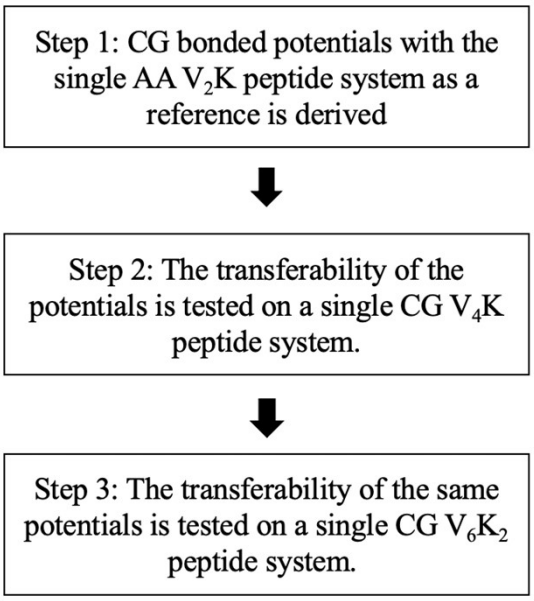


Figure SI.7: Increasing the peptide chain length from V_2K to V_6K_2. At every step, corrections are made to the set of CG potentials, and the updated set of CG potentials are transferred to the subsequent step.

Schematic representations of CG bonds:

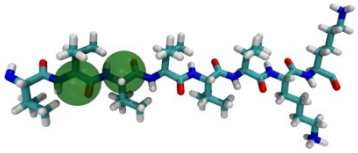
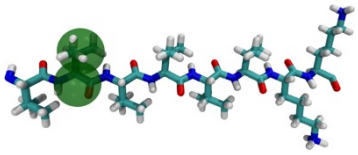
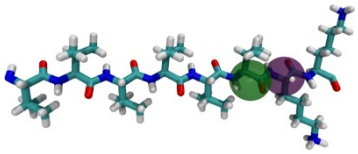
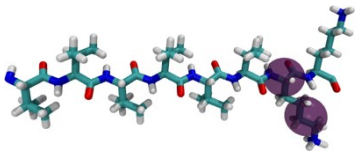
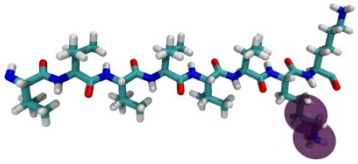
Type of Bonded Interaction	Name	Schematic Representation
Valine Backbone Bond	V_{Bx}-$V_{B(x+1)}$	
Valine Side chain Bond	V_{Bx}-V_{Sx}	
Valine-Lysine Connector Bond	V_{Bx}-K_{By}	
Lysine Long Bond	K_{By}-K_{Sy1}	
Lysine Short Bond	K_{Sy1}-K_{Sy2}	

Table SI.1: Schematic representations of V_6K_2 bonds reported in Figure 5.

Comparison of angle distributions between the AA and CG representations of the V_6K_2 peptide:

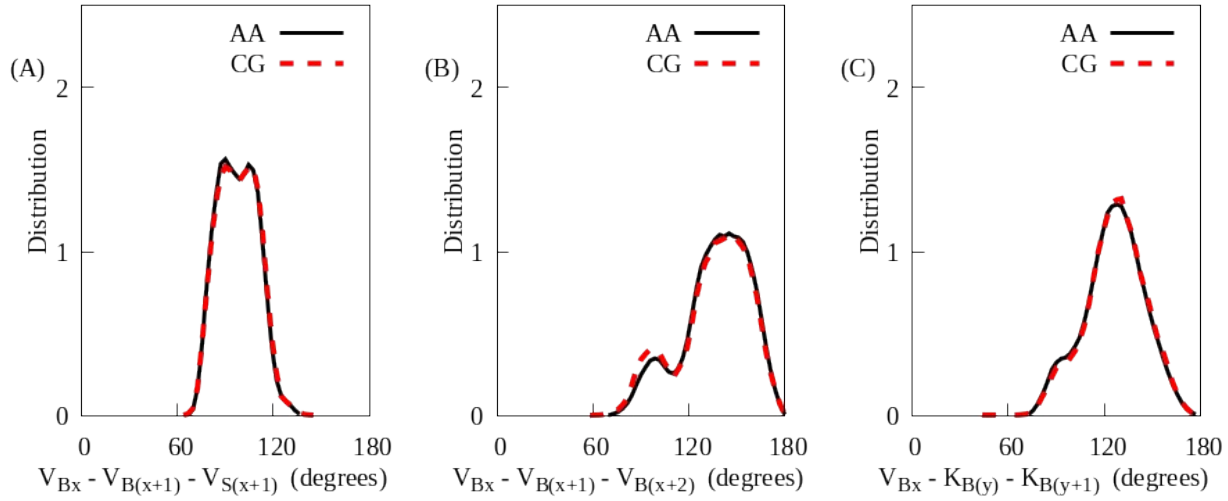


Fig. SI.8: Comparison of the reference (black) and CG (red) distributions for selected angles in the V_6K_2 peptide sequence.

Comparison of dihedral distributions between the AA and CG representations of the V_6K_2 peptide:

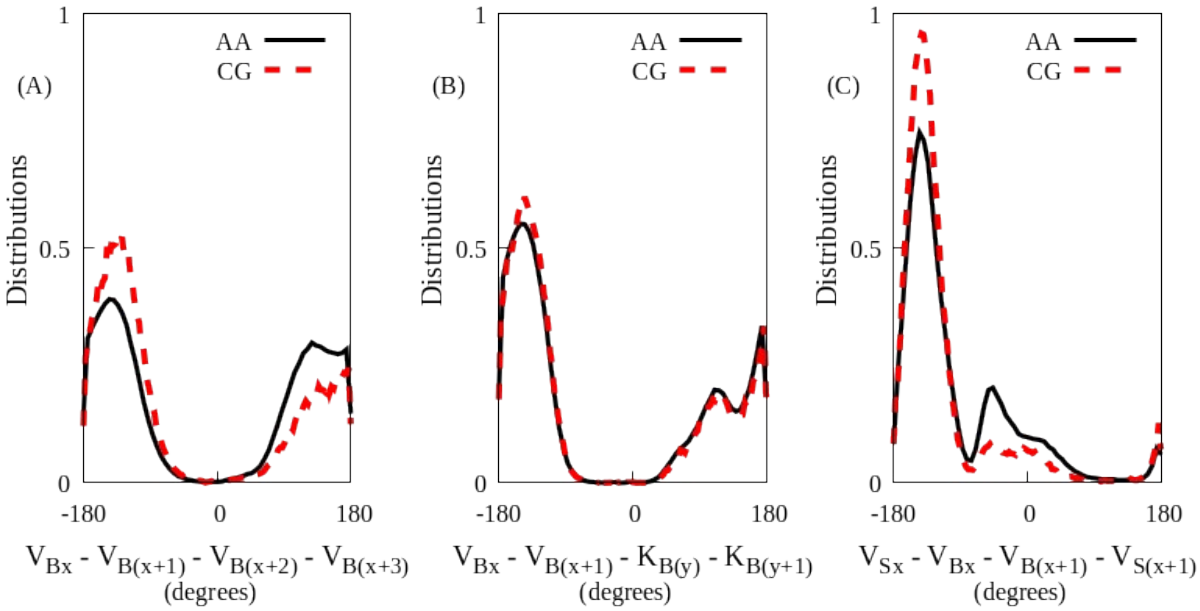


Fig. SI.9: Comparison of the reference (black) and CG (red) distributions for selected dihedrals in the V_6K_2 peptide sequence.

Intermolecular peptide-peptide and peptide-ion RDFs for the 25 V_2K peptide system:

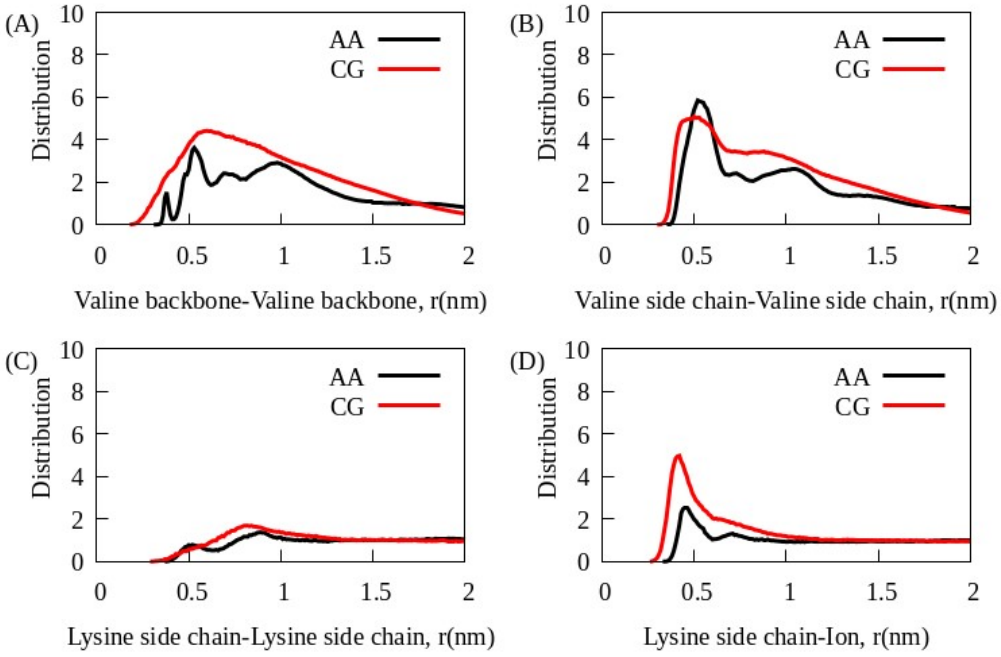


Fig. SI.10: Comparison of the reference (black) and CG (red) distributions for selected peptide-peptide and peptide-ion RDFs in the 25 V_2K peptide system. This comparison demonstrates the quality of the peptide-peptide and peptide-ion potentials obtained via FM.

Comparison of peptide conformation prior to addition of 1-3-5 angle potentials:

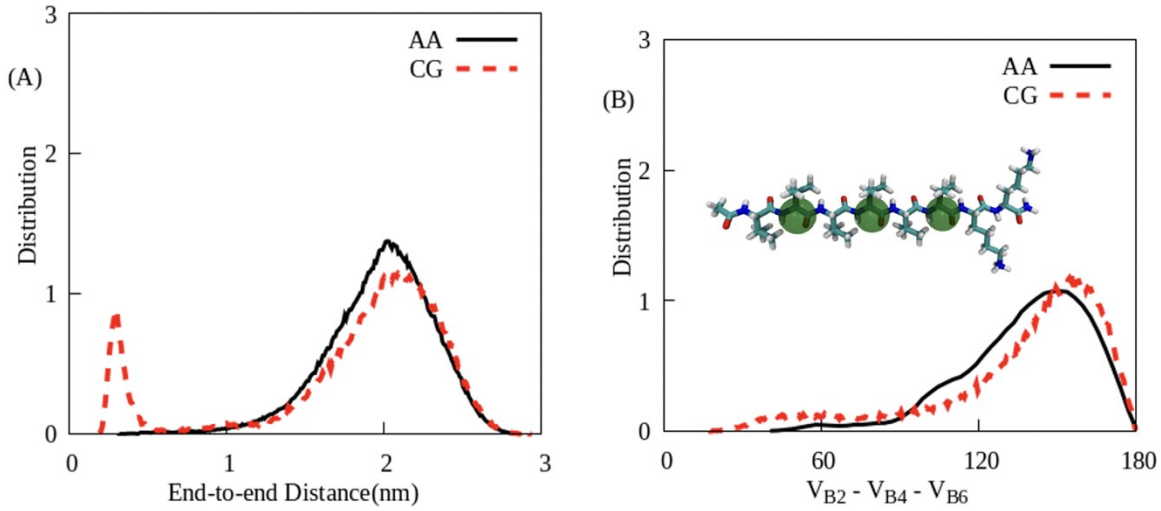


Fig. SI.11: The (A) end-to-end distance and a (B) selected 1-3-5 angle in a V_6K_2 peptide. The inset in (B) shows the CG representation of the 1-3-5 angle overlaid on the AA representation of the entire peptide sequence. The black and red curves represent AA and CG distributions, respectively.

Comparison of radius of gyration for the AA and CG representation of the V_6K_2 peptide:

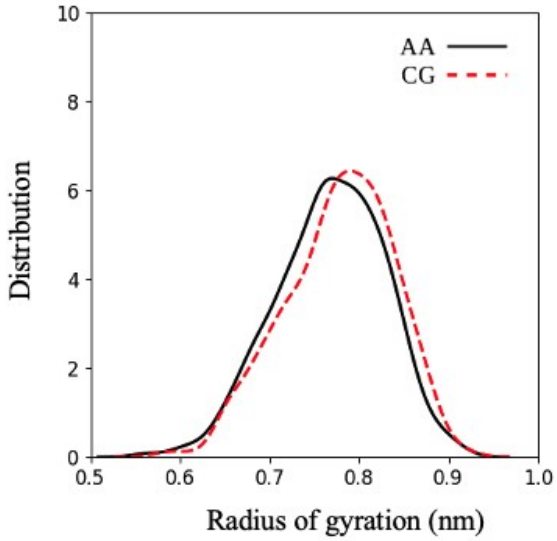


Fig. SI.12: Comparison of the radius of gyration for the AA (black) and CG (red) representations of the V_6K_2 peptide.

Comparison of internal structural properties for the AA and CG V_6K_2 peptide:

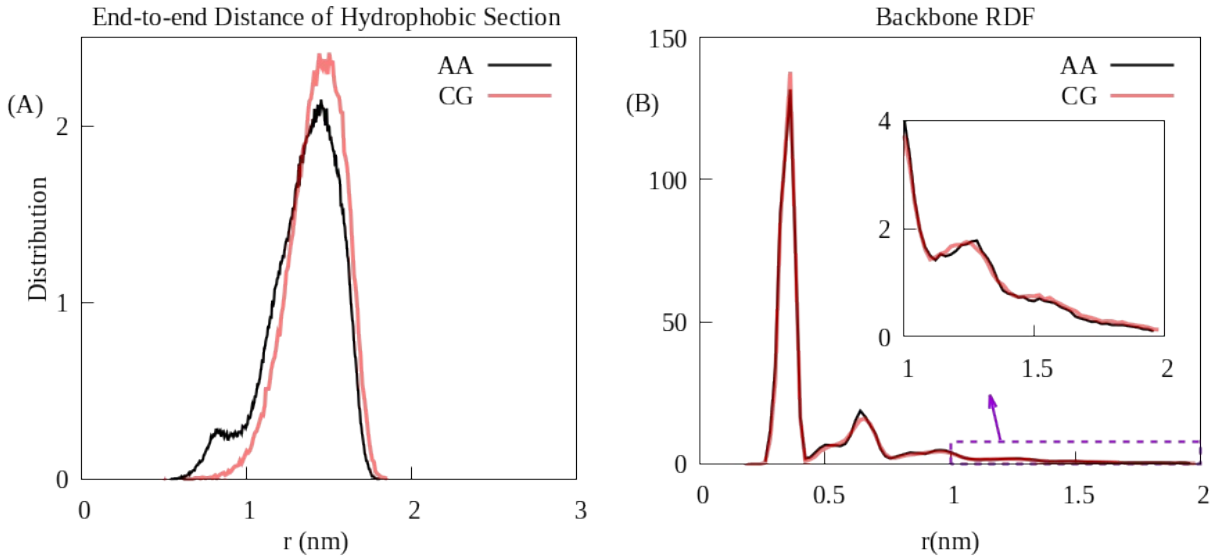


Fig. SI.13: A) The distance between the first and last Valine residues in the V_6K_2 peptide sequence. B) The radial distribution function of the backbone residues in a V_6K_2 peptide. Inset: Zoomed-in section of the RDF between r = 1 nm and 2 nm. The black and red curves represent AA and CG distributions, respectively.

Comparison of AA and CG Time Scales:

System	D_{CG} (10^{-5} cm^2/s)	D_{AA} (10^{-5} cm^2/s)	D_{CG}/D_{AA}
1 V_6K_2 peptide in aqueous solution	0.31 ± 0.03	0.21 ± 0.04	~1.5

Table S1.2: Comparison of self-diffusion coefficients in AA and CG simulations. The Einstein relation [1] is fitted to the linear regime of the plot of the time evolution of the mean square displacement of the center of mass of a V_6K_2 peptide. The slope of the line provides the self-diffusion coefficient.

Gain in computational efficiency by coarse-graining:

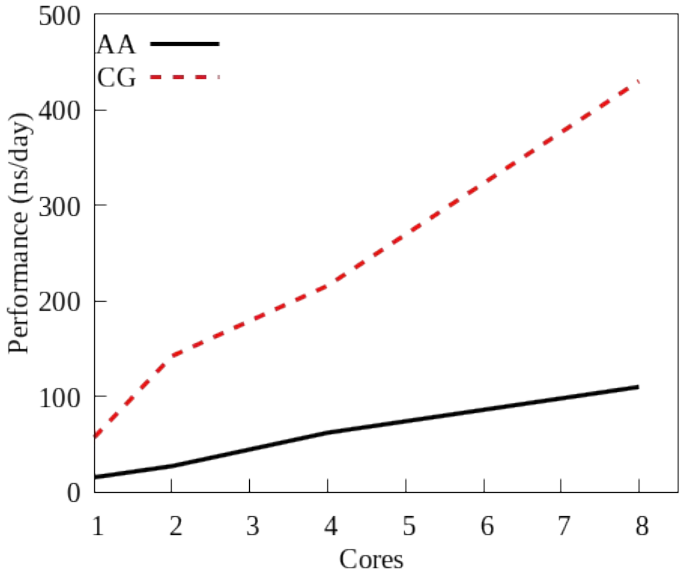


Figure SI.14: The performance of the AA and CG simulations are plotted as a function of the number of cores used on the supercomputer. The simulations were performed on Bridges2 at the Pittsburgh Supercomputing Center. An AMD EPYC 7742 CPU processor is used for these simulations. The scaling measurements are conducted on 1,2,4 and 8 cores on a CPU with a total of 64 cores.

Radius of gyration of peptides in multi-peptide systems:

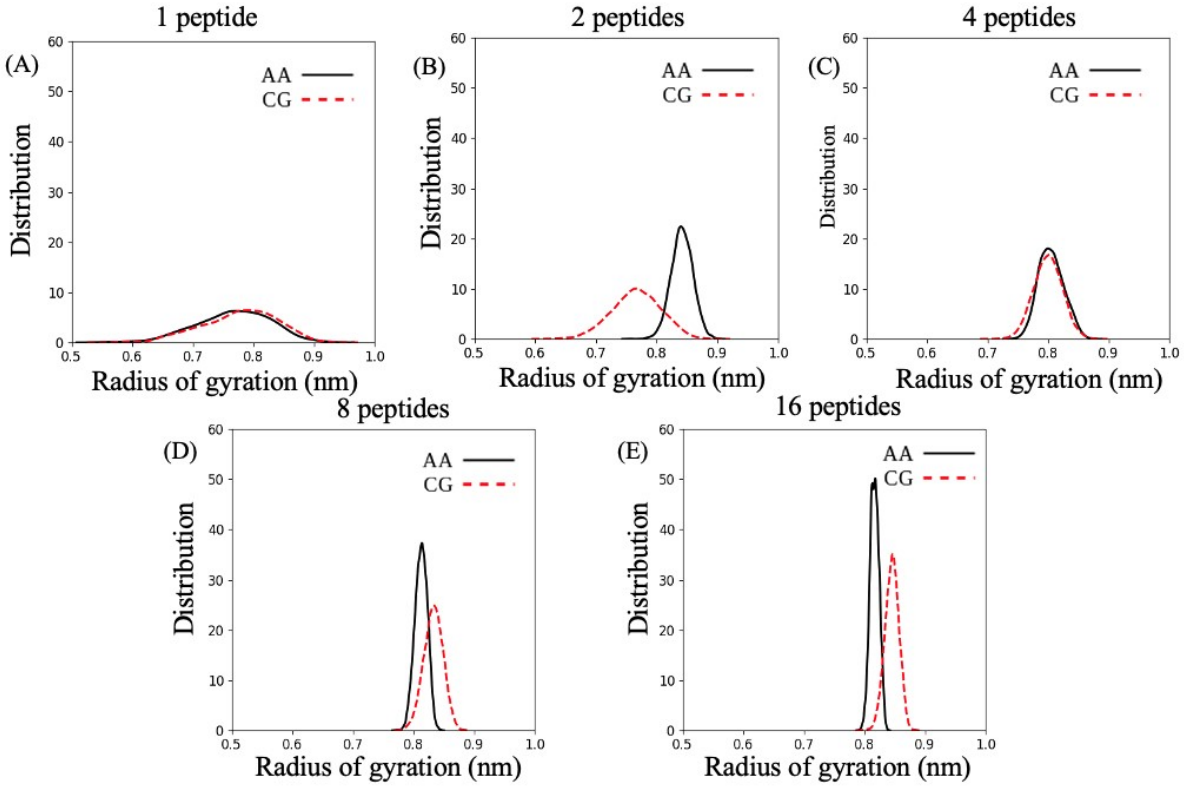


Fig. SI.15: The radius of gyration of peptides in the (A) 1, (B) 2, (C) 4, (D) 8 and (E) 16 peptide systems. The black and red curves represent AA and CG distributions, respectively.

Intermolecular RDFs of V_6K_2 peptides in multi-peptide simulations:

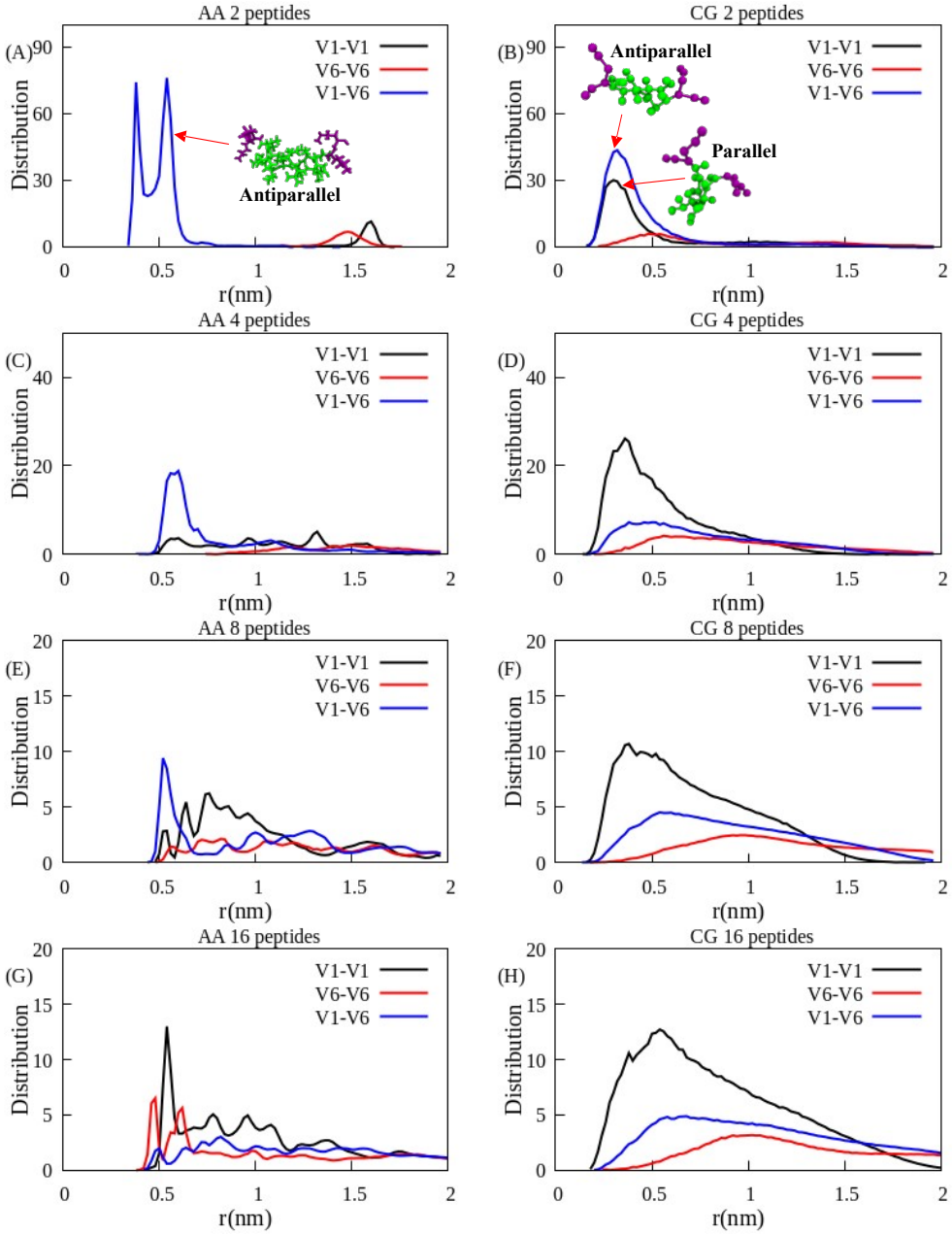


Figure SI.16: Intermolecular RDFs between first (V1) and last (V6) Valines in the V_6K_2 peptide sequence. (A, C, E and G) show the RDFs for the AA 2, 4, 8 and 16 peptide systems, respectively. (B, D, F and H) show the RDFs for the corresponding CG systems. The insets in (A) and (B) show

screenshots of the parallel and antiparallel orientation between 2 peptides. Color scheme – Green: Valine and Purple: Lysine.

Contact Maps:

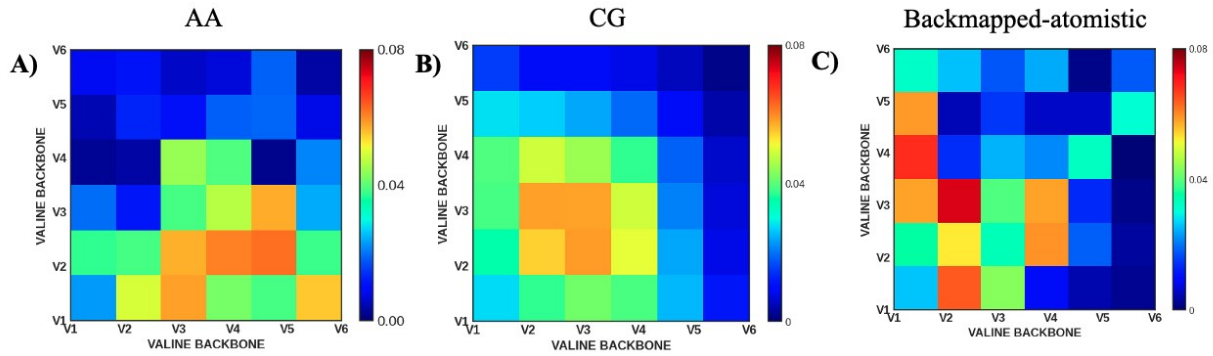


Fig. SI.17: Contact maps representing interpeptide interactions in 8 peptide systems. V1 represents the Valine residue that is farthest from the Lysine residues. Whereas V6 represents the Valine residue that is closest to the Lysine residues. The legend of the contact maps reports probability of the interactions which is given by the number of interactions between the two Valine residues within the cutoff distance/ total number of possible interactions between Valine residues. Red denotes a high probability of interaction and blue denotes a low probability of interaction.

Peptide-water interactions in a 8 peptide system across three resolutions:

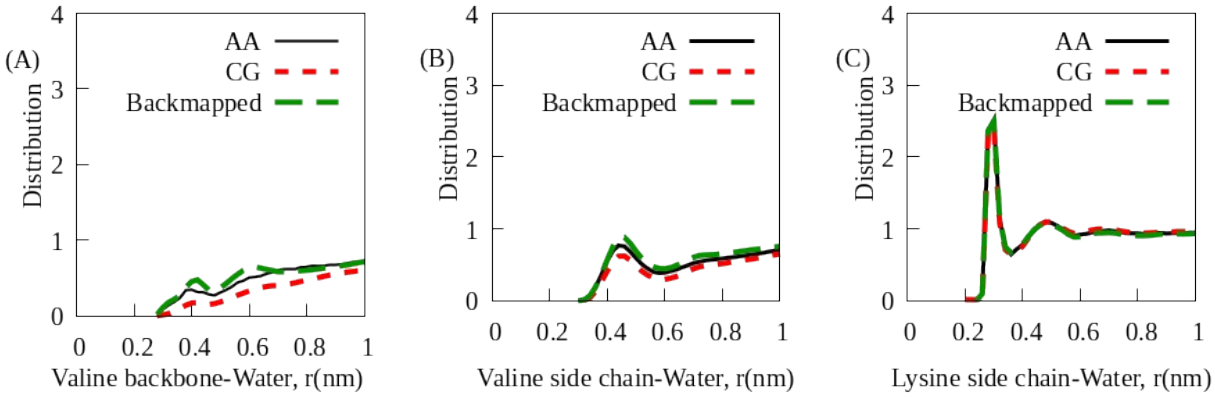


Figure SI.18: Black, red and green curves represent peptide-water interactions in AA, CG and backmapped-atomistic simulations, respectively.

Comparison of effective size of the micelle in AA, CG and backmapped-atomistic configurations:

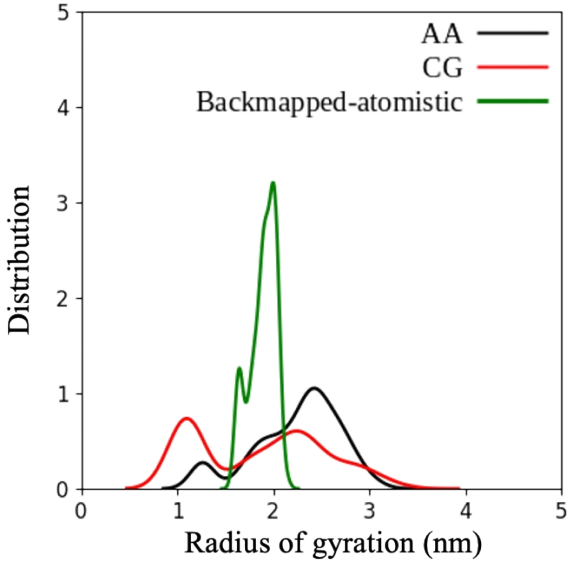


Fig. SI.19: Comparison of the radius of gyration for the AA (black), CG (red) and backmapped-atomistic (green) representations of the micelle formed in the 8 peptide system.

References:

1. M.P. Allen and D.J. Tildesley, *Computer simulations of liquids*. Oxford Science Publications, Oxford, 1987