Suppoting Information for
Improving Internal Peptide Dynamics in the Coarse-Grained MARTINI Model: Towards Large-Scale Simulations of Amyloid-like and Elastin-like Peptides

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Figure S11. Backbone dihedral angle probability distributions $P(\psi)$ for (GA)$_4$ from atomistic simulations. X-axis represents dihedral angle, $\psi$ in deg. The probability distribution of the dihedral angle is computed for the first half (blue), the second half (red), and the complete trajectory (purple).
Figure S11. (Continued) $P(\psi)$ for SNNFGAIL.
Figure SI1. (Continued) $P(\psi)$ for GVGVAGGV.
Figure SI1. (Continued) $P(\psi)$ for GVGVPGVG.
Figure S12. Backbone dihedral angle probability distributions $P(\psi)$ for $(GA)_4$ from CG simulations. The probability distribution of the dihedral angle is computed for the first half (black), the second half (red), and the complete trajectory (green).
Figure S12. (Continued) $P(\psi)$ for SNNFGAIL.
Figure S12. (Continued) $P(\psi)$ for GVGVAGGV.
Figure S12. (Continued) \( P(\psi) \) for GVGVPGVG.
Figure S13. The potentials of mean force (solid lines) and fitting energy functions (dotted lines) for all possible backbone dihedral angles of octapeptides. The potentials of mean force were extracted from the probability distributions of the dihedral angles calculated from atomistic trajectories.
Figure S13. Continued.
Table SI1. Derived dihedral CG parameters for tetrapeptides (Eq. 6 of the main document). K_i is given in kJ mol^{-1} nm^{-2} and φ_i in deg. n_i is multiplicity.

| i | φ_i  | K_i     | n_i | φ_i  | K_i     | n_i |
|---|------|---------|-----|------|---------|-----|
| 0 | 0.000000 | -0.107029 | 1   | 0.000000 | -0.387198 | 1   |
| 1 | 0.000000 | -0.240789 | 2   | 0.000000 | 0.141459  | 2   |
| 2 | 0.000000 | -0.045847 | 3   | 0.000000 | 0.123831  | 3   |
| 3 | 0.000000 | 0.088616  | 4   | 0.000000 | 0.116407  | 4   |
| 4 | 90.000000 | -2.259989 | 1   | 90.000000 | 0.323073  | 1   |
| 5 | 90.000000 | -0.293574 | 2   | 90.000000 | -0.172202 | 2   |
| 6 | 90.000000 | 0.371547  | 3   | 90.000000 | -0.113024 | 3   |
| 7 | 90.000000 | 0.303240  | 4   | 90.000000 | -0.079454 | 4   |
| 8 | 90.000000 | 17.612248 | 0   | 90.000000 | 14.999226 | 0   |

| i | φ_i  | K_i     | n_i | φ_i  | K_i     | n_i |
|---|------|---------|-----|------|---------|-----|
| 0 | 0.000000 | 0.612189 | 1   | 0.000000 | -1.557552 | 1   |
| 1 | 0.000000 | -0.489914 | 2   | 0.000000 | -0.454846 | 2   |
| 2 | 0.000000 | 0.140617  | 3   | 0.000000 | 0.390049  | 3   |
| 3 | 0.000000 | 0.129995  | 4   | 0.000000 | 0.345011  | 4   |
| 4 | 90.000000 | -2.648496 | 1   | 90.000000 | 1.056192  | 1   |
| 5 | 90.000000 | -0.026237 | 2   | 90.000000 | -0.026963 | 2   |
| 6 | 90.000000 | 0.391829  | 3   | 90.000000 | -0.079454 | 3   |
| 7 | 90.000000 | 0.220901  | 4   | 90.000000 | -0.294953 | 4   |
| 8 | 90.000000 | 17.305153 | 0   | 90.000000 | 16.540000 | 0   |

| i | φ_i  | K_i     | n_i | φ_i  | K_i     | n_i |
|---|------|---------|-----|------|---------|-----|
| 0 | 0.000000 | 0.282397 | 1   | 0.000000 | -1.140736 | 1   |
| 1 | 0.000000 | -0.093562 | 2   | 0.000000 | -0.017667 | 2   |
| 2 | 0.000000 | 0.184967  | 3   | 0.000000 | 0.088631  | 3   |
| 3 | 0.000000 | 0.110376  | 4   | 0.000000 | 0.196805  | 4   |
| 4 | 90.000000 | -2.826619 | 1   | 90.000000 | 0.336172  | 1   |
| 5 | 90.000000 | -0.976492 | 2   | 90.000000 | -0.279399 | 2   |
| 6 | 90.000000 | 0.187278  | 3   | 90.000000 | -0.100757 | 3   |
| 7 | 90.000000 | 0.117143  | 4   | 90.000000 | -0.306441 | 4   |
| 8 | 90.000000 | 18.778401 | 0   | 90.000000 | 16.281485 | 0   |

| i | φ_i  | K_i     | n_i | φ_i  | K_i     | n_i |
|---|------|---------|-----|------|---------|-----|
| 0 | 0.000000 | 3.039320 | 1   | 0.000000 | 2.471758 | 1   |
| 1 | 0.000000 | 0.954368 | 2   | 0.000000 | 0.510827 | 2   |
| 2 | 0.000000 | -0.371006 | 3   | 0.000000 | 0.569905 | 3   |
| 3 | 0.000000 | -0.271769 | 4   | 0.000000 | 0.231177 | 4   |
| 4 | 90.000000 | -1.915955 | 1   | 90.000000 | -2.905913 | 1   |
| 5 | 90.000000 | -1.599522 | 2   | 90.000000 | -1.108903 | 2   |
| 6 | 90.000000 | 0.289154  | 3   | 90.000000 | 0.184505  | 3   |
| 7 | 90.000000 | 0.142438  | 4   | 90.000000 | 0.395382  | 4   |
| 8 | 90.000000 | 15.960449 | 0   | 90.000000 | 15.963075 | 0   |
Table SII. Continued.

| i  | $\phi_i$ | $K_i$  | $n_i$ | $\phi_i$ | $K_i$  | $n_i$ |
|----|---------|-------|------|---------|-------|------|
| 0  | 0.000000| 0.976996| 1    | 0.000000| 3.482771| 1    |
| 1  | 0.000000| 0.050850| 2    | 0.000000| 2.147892| 2    |
| 2  | 0.000000| -0.756830| 3   | 0.000000| -0.125944| 3    |
| 3  | 0.000000| 0.168020| 4    | 0.000000| 0.074559| 4    |
| 4  | 90.000000| -0.850899| 1   | 90.000000| -0.329573| 1    |
| 5  | 90.000000| -0.796810| 2   | 90.000000| -1.029307| 2    |
| 6  | 90.000000| 0.231184| 3    | 90.000000| 0.557539| 3    |
| 7  | 90.000000| 0.182909| 4    | 90.000000| 0.140045| 4    |
| 8  | 90.000000| 15.983796| 0   | 90.000000| 11.323095| 0    |
| 0  | 0.000000| -0.402009| 1   | 0.000000| -0.185406| 1    |
| 1  | 0.000000| 0.021694| 2    | 0.000000| -0.184531| 2    |
| 2  | 0.000000| -0.165141| 3   | 0.000000| 0.042111| 3    |
| 3  | 0.000000| 0.011021| 4    | 0.000000| 0.055186| 4    |
| 4  | 90.000000| 0.114472| 1    | 90.000000| 0.195645| 1    |
| 5  | 90.000000| -0.256438| 2   | 90.000000| -0.530603| 2    |
| 6  | 90.000000| 0.141132| 3    | 90.000000| -0.033636| 3    |
| 7  | 90.000000| -0.393561| 4   | 90.000000| -0.312372| 4    |
| 8  | 90.000000| 15.886439| 0   | 90.000000| 15.953331| 0    |
| 0  | 0.000000| 3.404023| 1    | 0.000000| -0.636232| 1    |
| 1  | 0.000000| 1.517194| 2    | 0.000000| 0.062710| 2    |
| 2  | 0.000000| -0.151486| 3   | 0.000000| -0.007445| 3    |
| 3  | 0.000000| 0.003505| 4    | 0.000000| 0.445799| 4    |
| 4  | 90.000000| 4.898950| 1    | 90.000000| -0.016874| 1    |
| 5  | 90.000000| -1.246595| 2   | 90.000000| -0.232684| 2    |
| 6  | 90.000000| -0.587647| 3   | 90.000000| 0.014639| 3    |
| 7  | 90.000000| -0.123101| 4   | 90.000000| -0.221027| 4    |
| 8  | 90.000000| 10.868441| 0   | 90.000000| 15.560684| 0    |
| 0  | 0.000000| 1.858642| 1    | 0.000000| 0.746513| 1    |
| 1  | 0.000000| -0.139087| 2   | 0.000000| -0.332803| 2    |
| 2  | 0.000000| -0.874251| 3   | 0.000000| 0.046517| 3    |
| 3  | 0.000000| 0.186661| 4    | 0.000000| 0.105136| 4    |
| 4  | 90.000000| -3.303938| 1   | 90.000000| -2.617351| 1    |
| 5  | 90.000000| -1.135280| 2   | 90.000000| -0.161660| 2    |
| 6  | 90.000000| -0.048363| 3   | 90.000000| 0.468383| 3    |
| 7  | 90.000000| -0.168022| 4   | 90.000000| 0.259117| 4    |
| 8  | 90.000000| 19.774256| 0   | 90.000000| 17.127026| 0    |
Table S11. Continued.

| i | $\phi$ | $K$ | $n$ | $\phi$ | $K$ | $n$ |
|---|---|---|---|---|---|---|
| 0 | 0.000000 | 2.815029 | 1 | 0.000000 | 3.810278 | 1 |
| 1 | 0.000000 | 0.426129 | 2 | 0.000000 | 0.682017 | 2 |
| 2 | 0.000000 | 0.674323 | 3 | 0.000000 | -0.132029 | 3 |
| 3 | 0.000000 | 0.437253 | 4 | 0.000000 | 0.210327 | 4 |
| 4 | 90.000000 | -3.080922 | 1 | 90.000000 | -1.518550 | 1 |
| 5 | 90.000000 | -0.824217 | 2 | 90.000000 | -1.398166 | 2 |
| 6 | 90.000000 | 0.014393 | 3 | 90.000000 | 0.543148 | 3 |
| 7 | 90.000000 | 0.449709 | 4 | 90.000000 | -0.004500 | 4 |
| 8 | 90.000000 | 15.593331 | 0 | 90.000000 | 14.295962 | 0 |

| 0 | 0.000000 | -0.714639 | 1 | 0.000000 | 3.081904 | 1 |
| 1 | 0.000000 | 0.019523 | 2 | 0.000000 | 1.800369 | 2 |
| 2 | 0.000000 | 0.099816 | 3 | 0.000000 | -0.375946 | 3 |
| 3 | 0.000000 | 0.405188 | 4 | 0.000000 | -0.092105 | 4 |
| 4 | 90.000000 | 0.374792 | 1 | 90.000000 | 0.529893 | 3 |
| 5 | 90.000000 | -0.337005 | 2 | 90.000000 | -0.049402 | 4 |
| 6 | 90.000000 | 4.383422 | 3 | 90.000000 | 10.929294 | 0 |
| 7 | 90.000000 | 0.267429 | 4 | 90.000000 | -0.004500 | 4 |
| 8 | 90.000000 | 15.933580 | 0 | 90.000000 | 14.295962 | 0 |

| 0 | 0.000000 | 0.405188 | 1 | 0.000000 | 0.068082 | 1 |
| 1 | 0.000000 | -0.464750 | 2 | 0.000000 | -0.459752 | 2 |
| 2 | 0.000000 | 0.131057 | 3 | 0.000000 | 0.321160 | 3 |
| 3 | 0.000000 | 0.113520 | 4 | 0.000000 | 0.138277 | 4 |
| 4 | 90.000000 | -2.498661 | 1 | 90.000000 | 4.062207 | 1 |
| 5 | 90.000000 | -0.011364 | 2 | 90.000000 | -0.070184 | 2 |
| 6 | 90.000000 | 0.480663 | 3 | 90.000000 | 0.665566 | 3 |
| 7 | 90.000000 | 0.267429 | 4 | 90.000000 | -0.418288 | 4 |
| 8 | 90.000000 | 17.134690 | 0 | 90.000000 | 12.047799 | 0 |

| 0 | 0.000000 | -0.970742 | 1 | 0.000000 | -0.970742 | 1 |
| 1 | 0.000000 | -0.421440 | 2 | 0.000000 | -0.421440 | 2 |
| 2 | 0.000000 | 0.314365 | 3 | 0.000000 | 0.314365 | 3 |
| 3 | 0.000000 | 0.473802 | 4 | 0.000000 | 0.473802 | 4 |
| 4 | 90.000000 | 1.152995 | 1 | 90.000000 | 1.152995 | 1 |
| 5 | 90.000000 | -0.597699 | 2 | 90.000000 | -0.597699 | 2 |
| 6 | 90.000000 | -0.148852 | 3 | 90.000000 | -0.148852 | 3 |
| 7 | 90.000000 | -0.461853 | 4 | 90.000000 | -0.461853 | 4 |
| 8 | 90.000000 | 15.893715 | 0 | 90.000000 | 15.893715 | 0 |