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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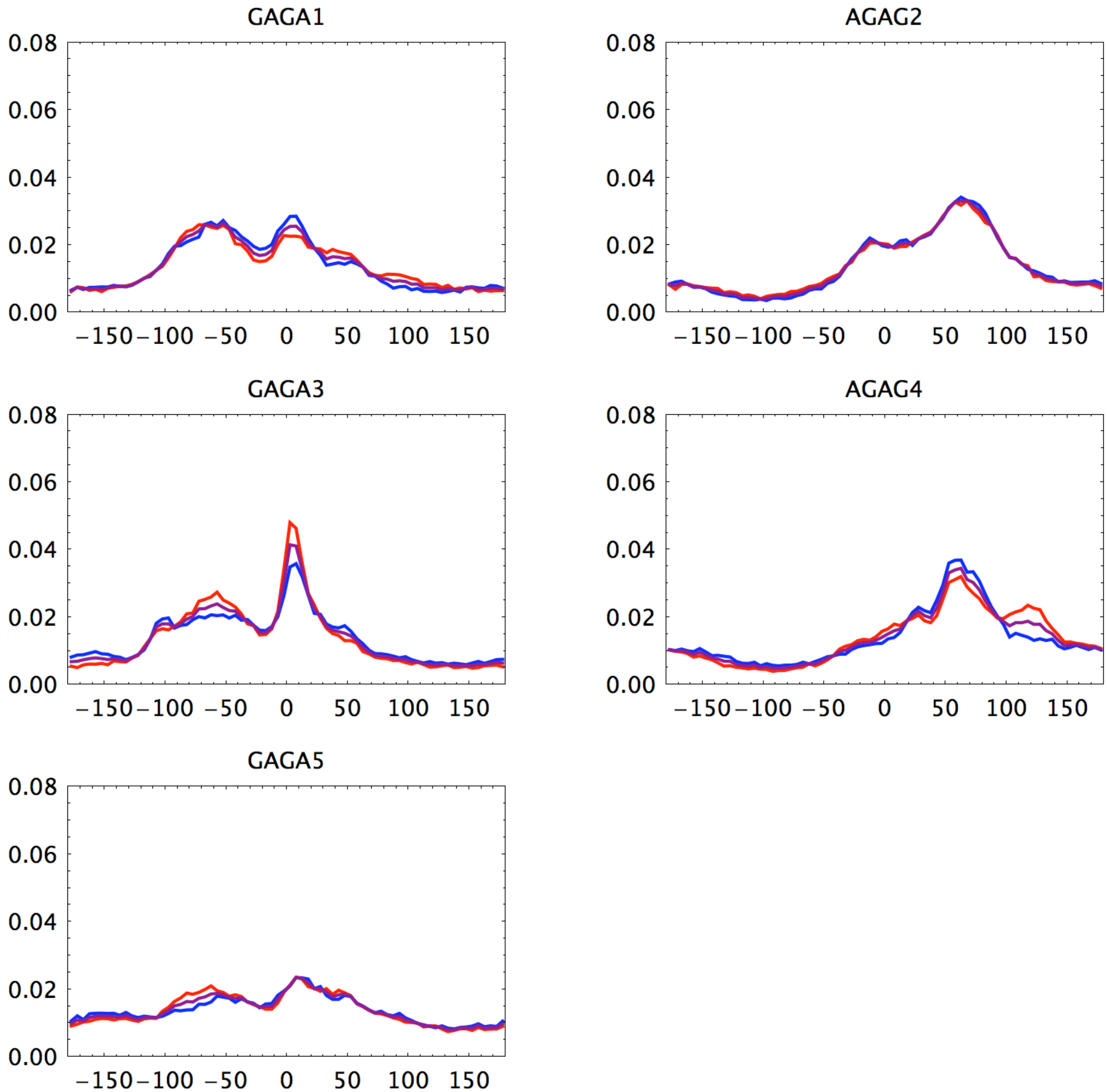

Figure SI1. Backbone dihedral angle probability distributions P(ψ) for $(GA)_4$ from atomistic simulations. X-axis represents dihedral angle, ψ in deg. The probability distribution of the dihedral angle is computed for the first half (blue), the second half (red), and the complete trajectory (purple).

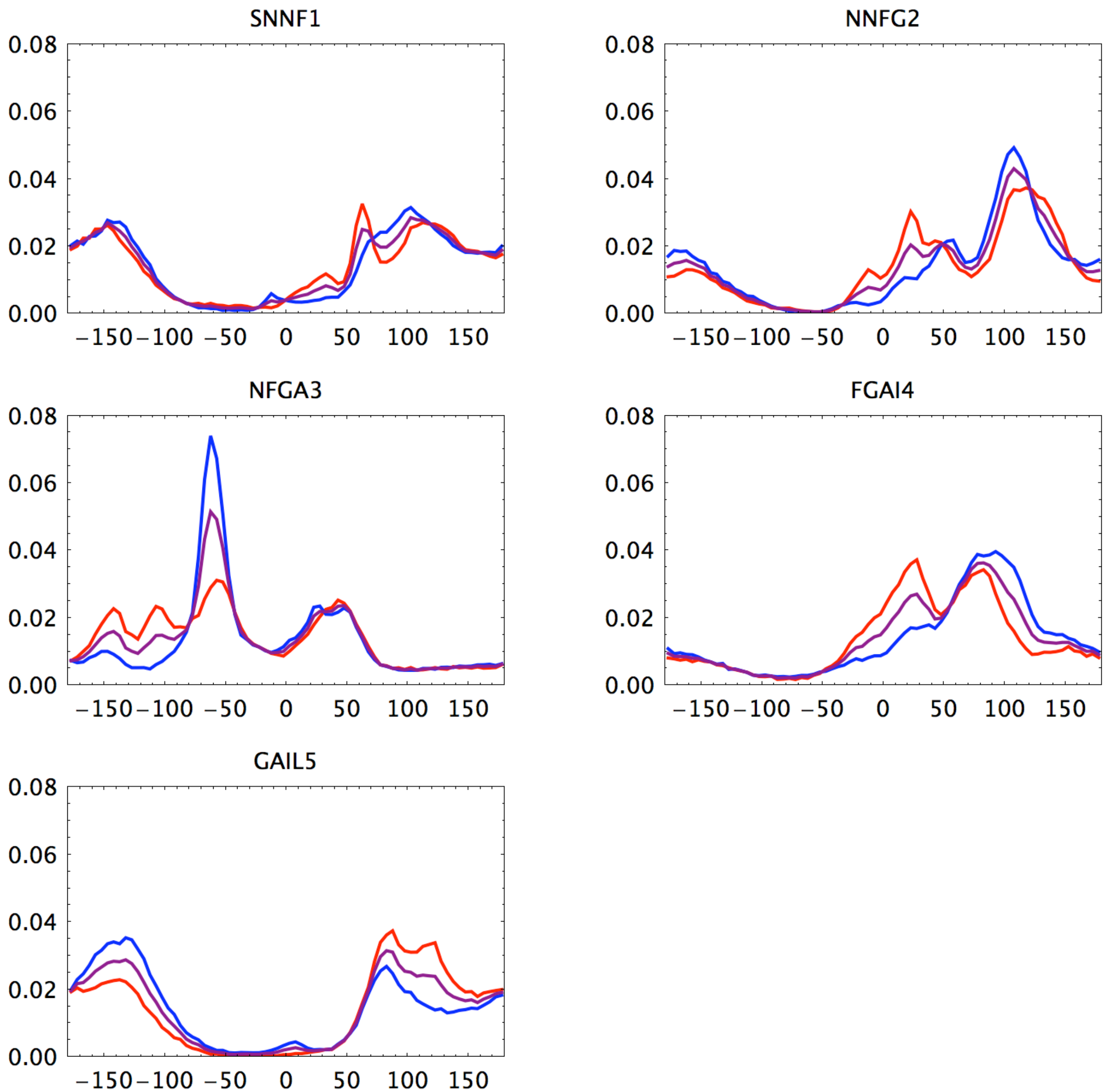

Figure SI1. (Continued) P(ψ) for SNNFGAIL.

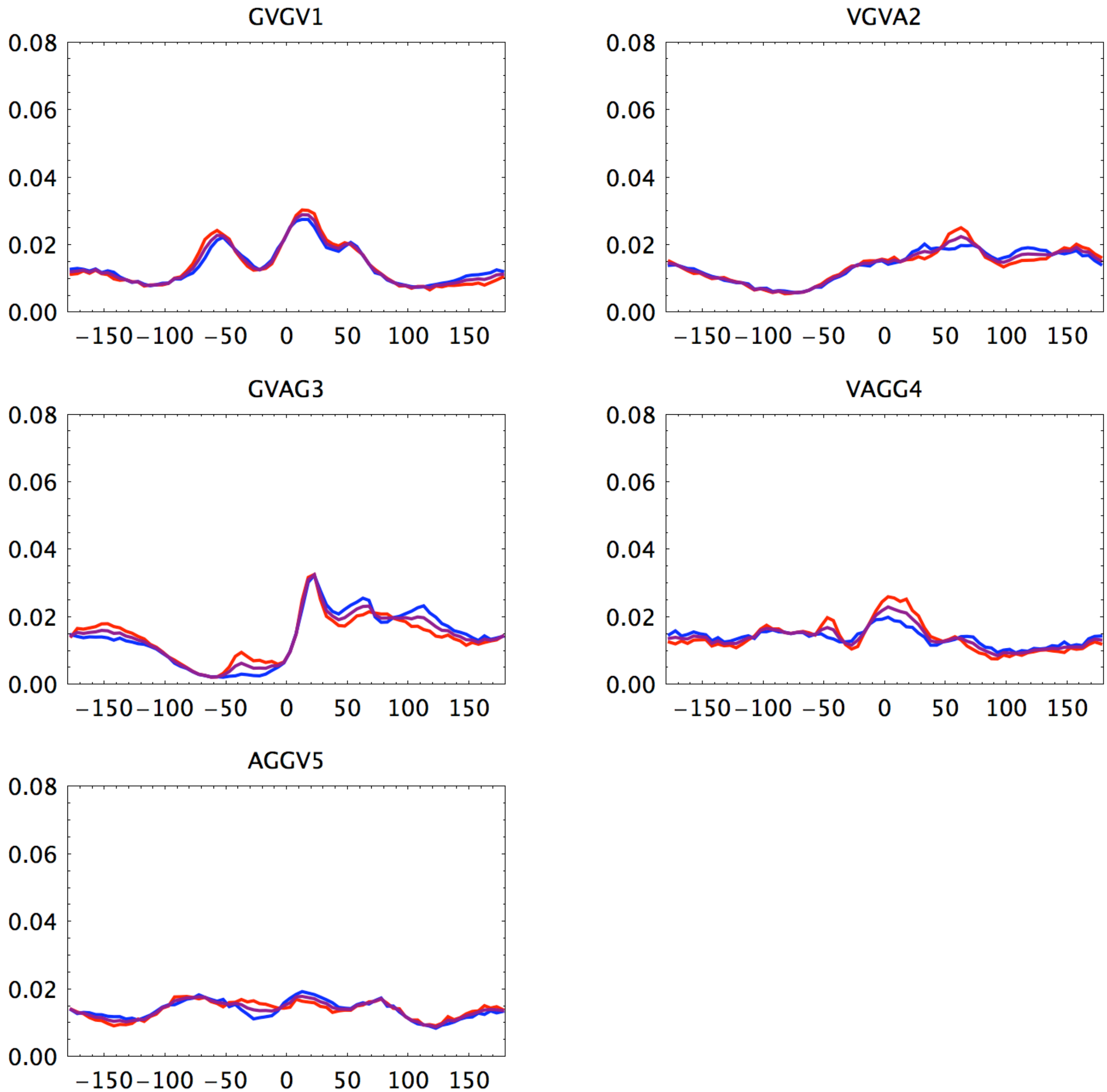

Figure SI1. (Continued) P(ψ) for GVGVAGGV.

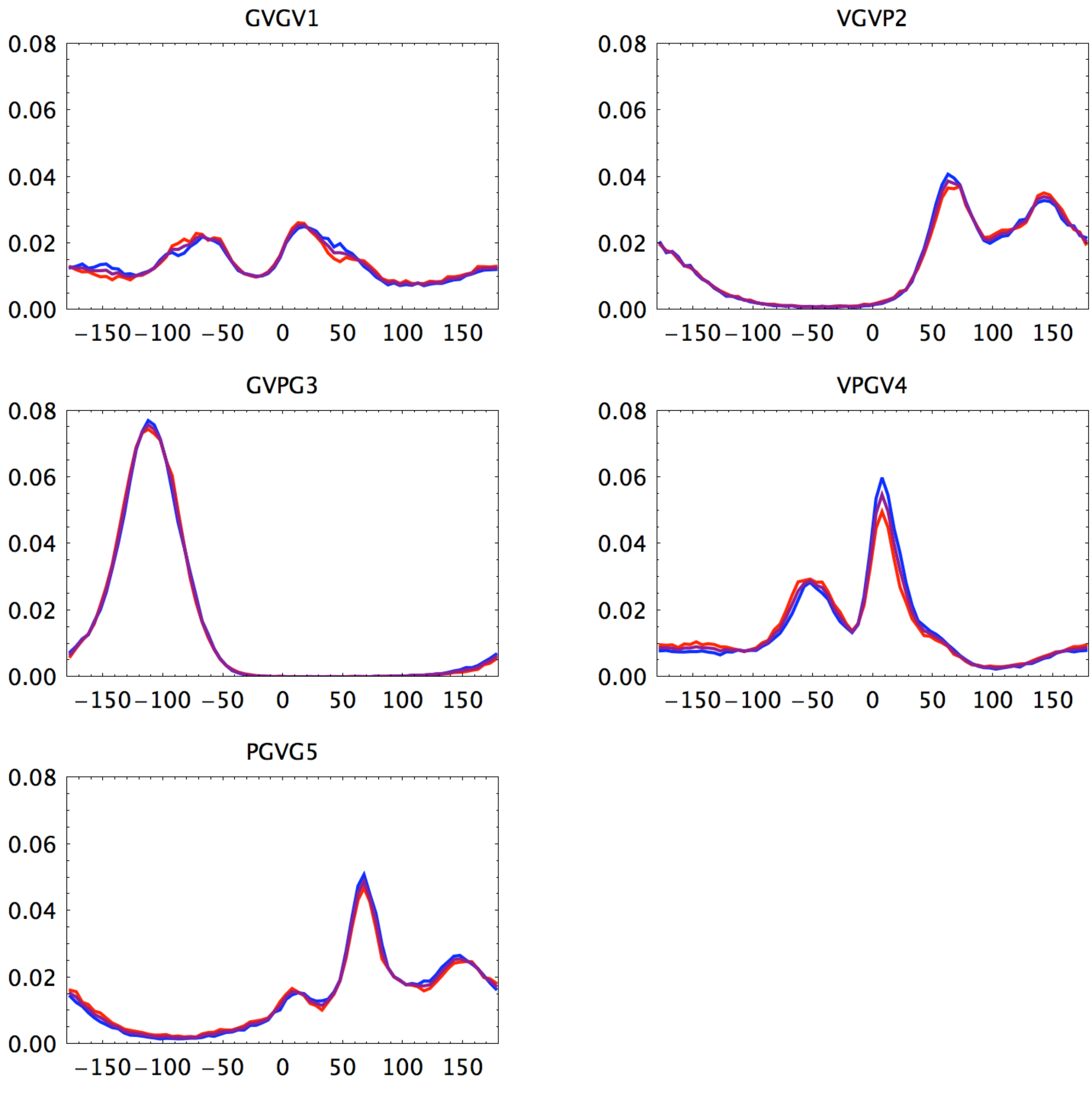

Figure SI1. (Continued) P(ψ) for GVGVPGVG.

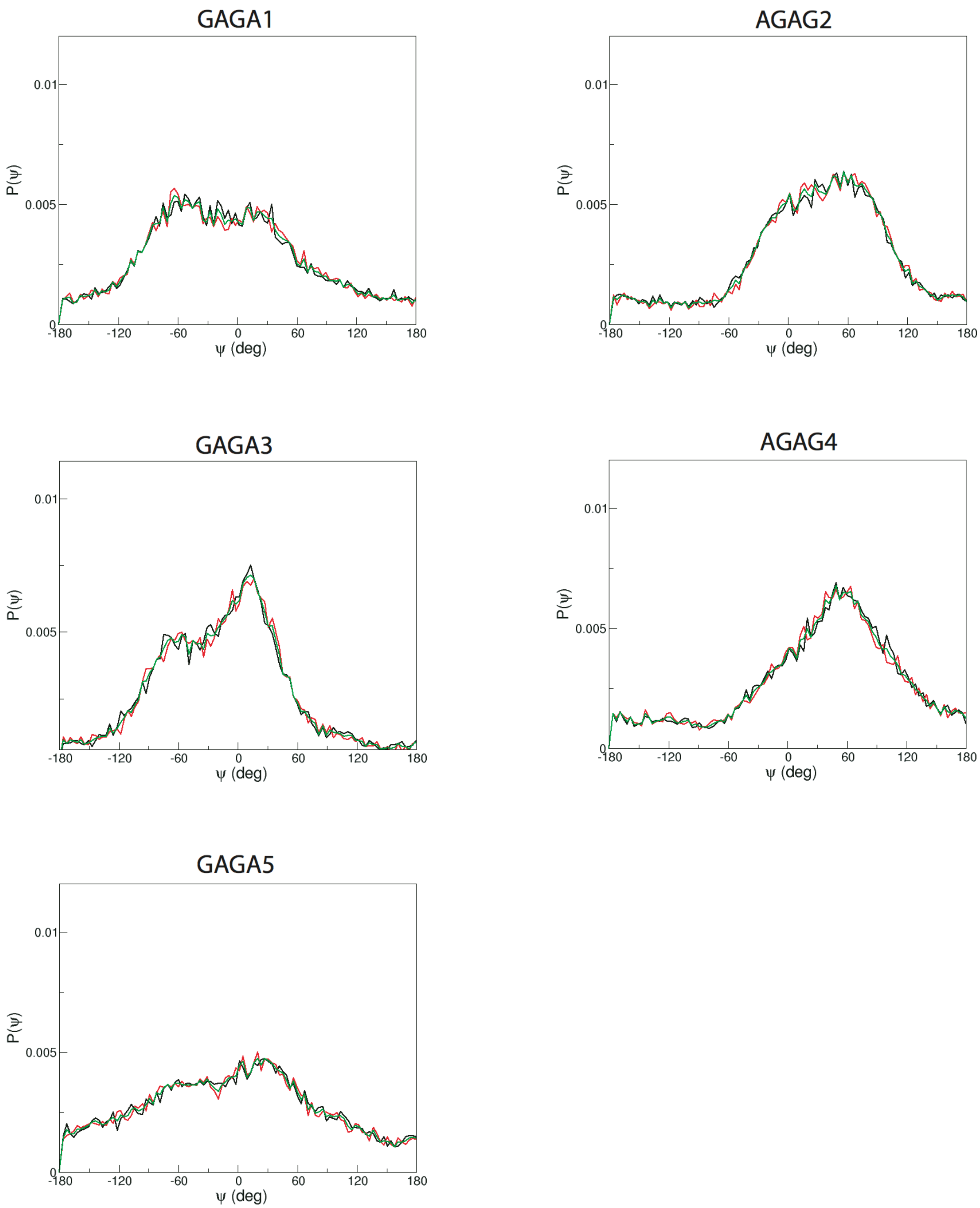

Figure SI2. Backbone dihedral angle probability distributions P(ψ) for $(GA)_4$ from CG simulations. The probability distribution of the dihedral angle is computed for the first half (black), the second half (red), and the complete trajectory (green).

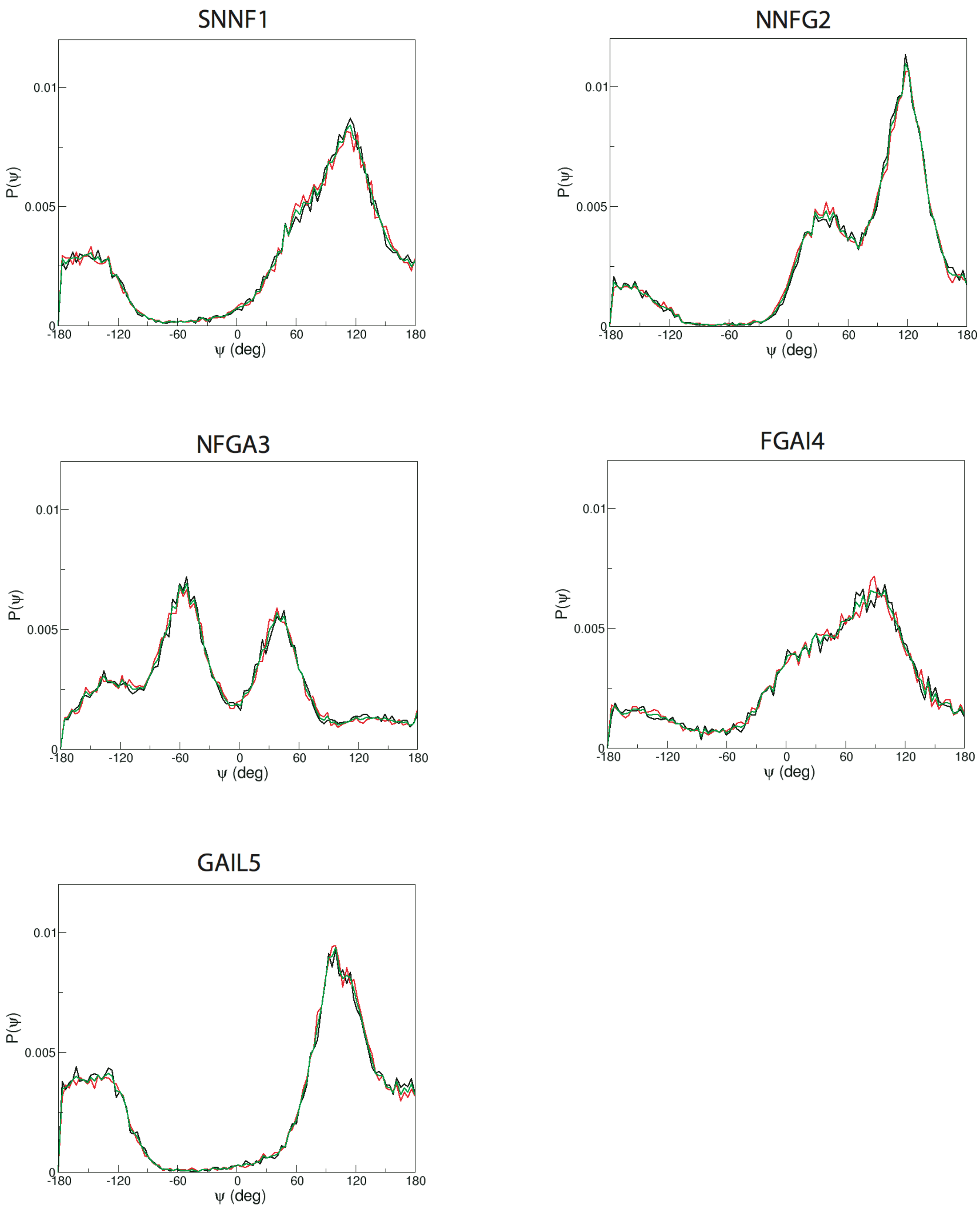

Figure SI2. (Continued) P(ψ) for SNNFGAIL.

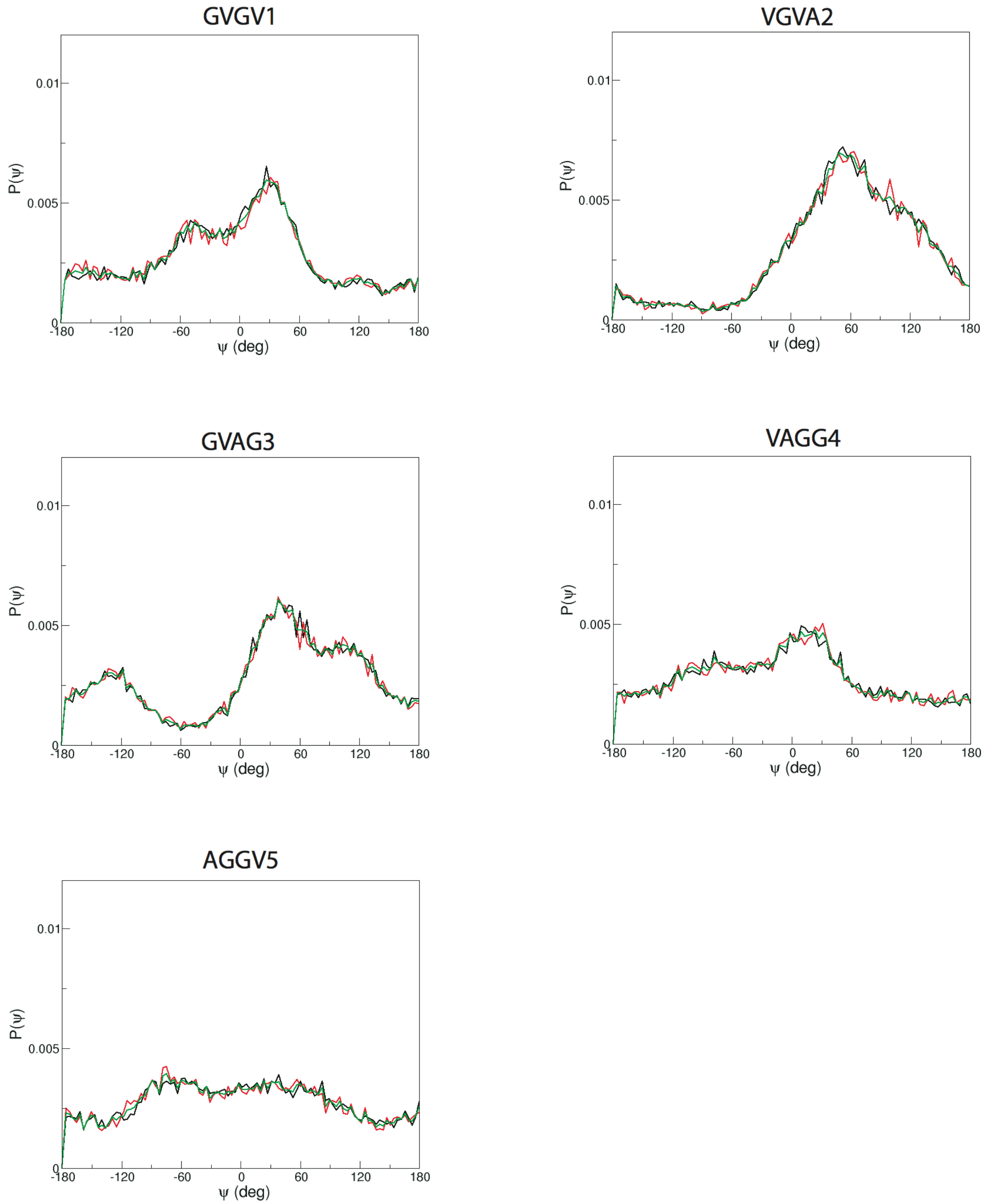

Figure SI2. (Continued) P(ψ) for GVGVAGGV.

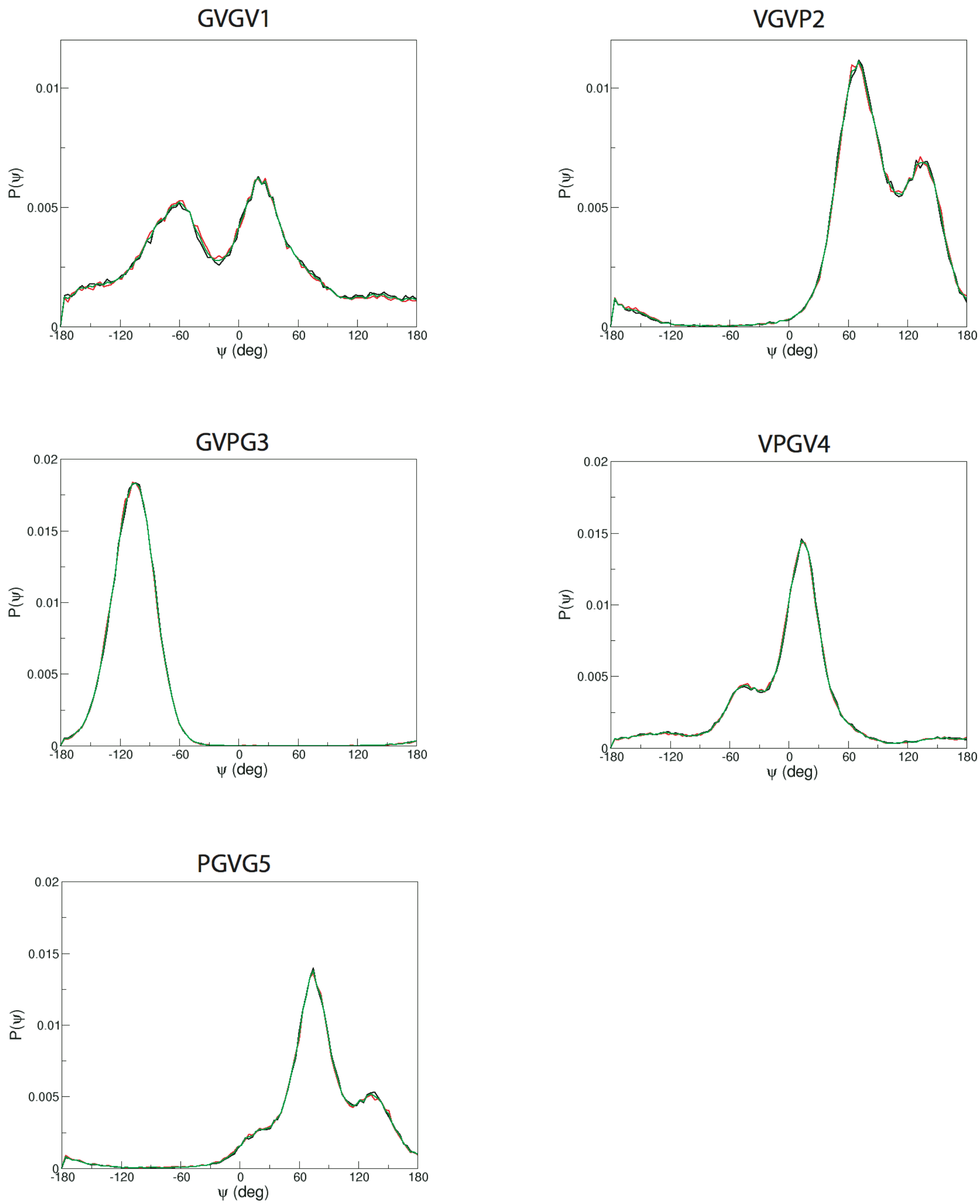

Figure SI2. (Continued) P(ψ) for GVGVPGVG.

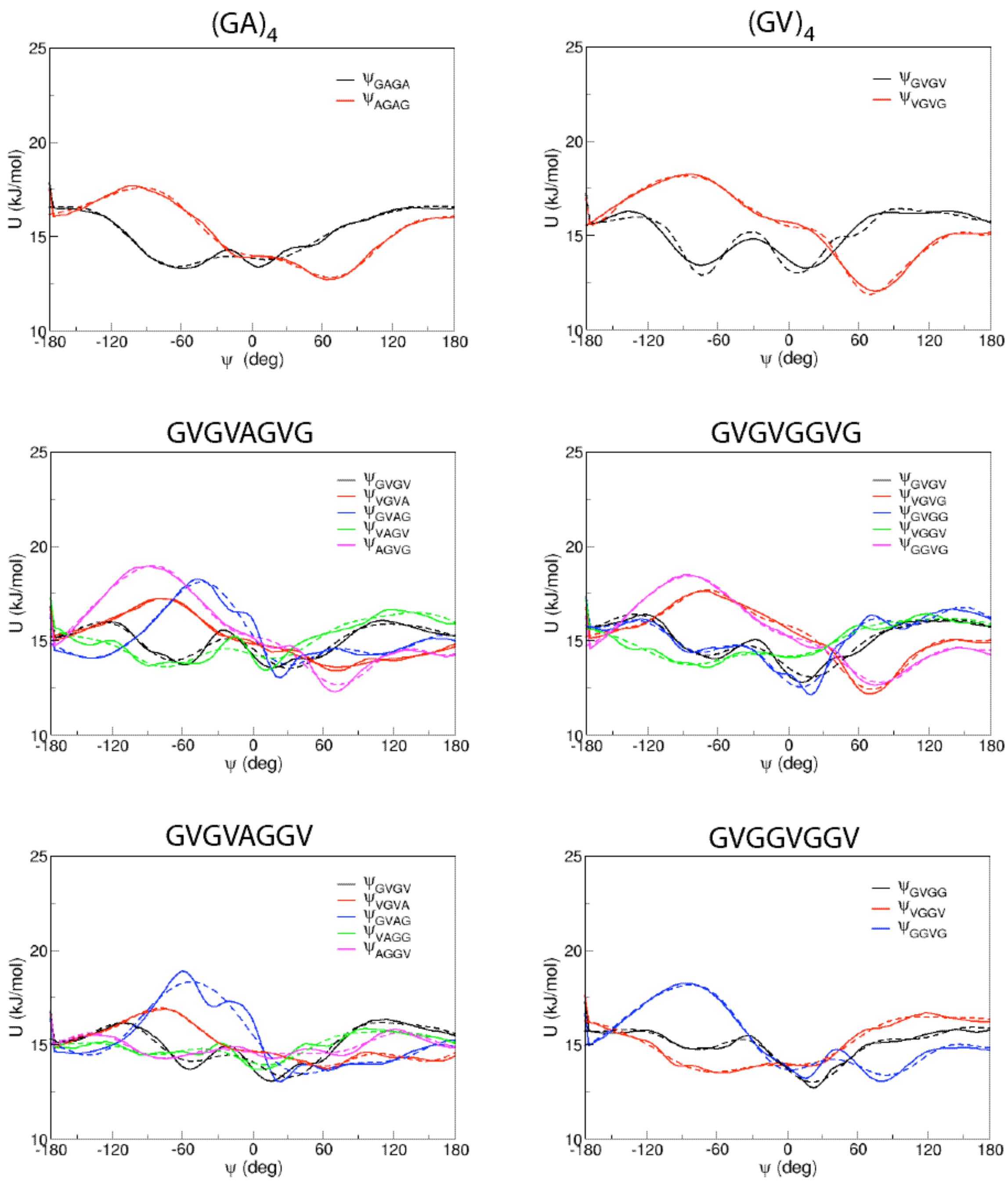

Figure SI3. The potentials of mean force (solid lines) and fitting energy functions (dotted lines) for all possible backbone dihedral angles of octapeptides. The potentials of mean force were extracted from the probability distributions of the dihedral angles calculated from atomistic trajectories.

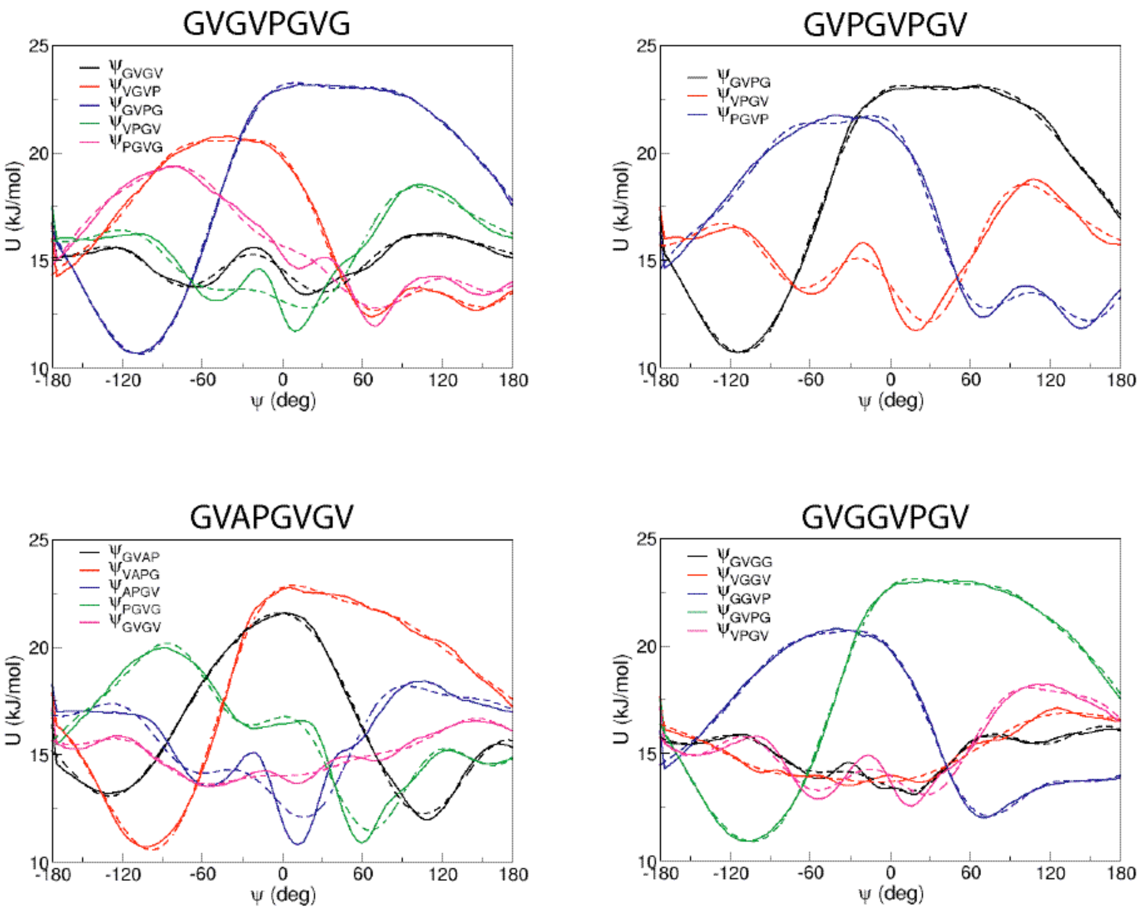

Figure SI3. Continued.

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
	ψ_{AGAG}			ψ_{AGGV}		
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
	ψ_{AGVG}			ψ_{APGV}		
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	-0.667619	2
6	90.000000	0.391829	3	90.000000	-0.026963	3
7	90.000000	0.220901	4	90.000000	-0.294953	4
8	90.000000	17.305153	0	90.000000	16.540000	0
	ψ_{FGAI}			ψ_{GAGA}		
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
	ψ_{GAIL}			ψ_{GGVP}		
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 SI1. Continued.

i	ϕ_i	K_i	n_i	ϕ_i	K_i	n_i
	ψ_{GVAG}			ψ_{GVAP}		
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
	ψ_{GVGG}			ψ_{GVGV}		
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
	ψ_{GVPG}			ψ_{NFGA}		
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
	ψ_{NNFG}			ψ_{PGVG}		
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 SI1. Continued.

i	ϕ_i	K_i	n_i	ϕ_i	K_i	n_i
	ψ_{PGVP}			ψ_{SNNF}		
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
	ψ_{VAGV}			ψ_{VAPG}		
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	0.044411	4	0.000000	-0.092105	4
4	90.000000	0.374792	1	90.000000	4.383422	1
5	90.000000	-0.337005	2	90.000000	-0.976558	2
6	90.000000	-0.001865	3	90.000000	-0.529893	3
7	90.000000	-0.405671	4	90.000000	-0.049402	4
8	90.000000	15.933580	0	90.000000	10.929294	0
	ψ_{VGVG}			ψ_{VGVP}		
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
	ψ_{VPGV}					
0	0.000000	-0.970742	1			
1	0.000000	-0.421440	2			
2	0.000000	0.314365	3			
3	0.000000	0.473802	4			
4	90.000000	1.152995	1			
5	90.000000	-0.597699	2			
6	90.000000	-0.148852	3			
7	90.000000	-0.461853	4			
8	90.000000	15.893715	0			