Supplementary materials

Effects of all-atom force fields on amyloid oligomerization: Replica exchange molecular dynamics simulations of the Aβ_{16-22} dimer and trimer

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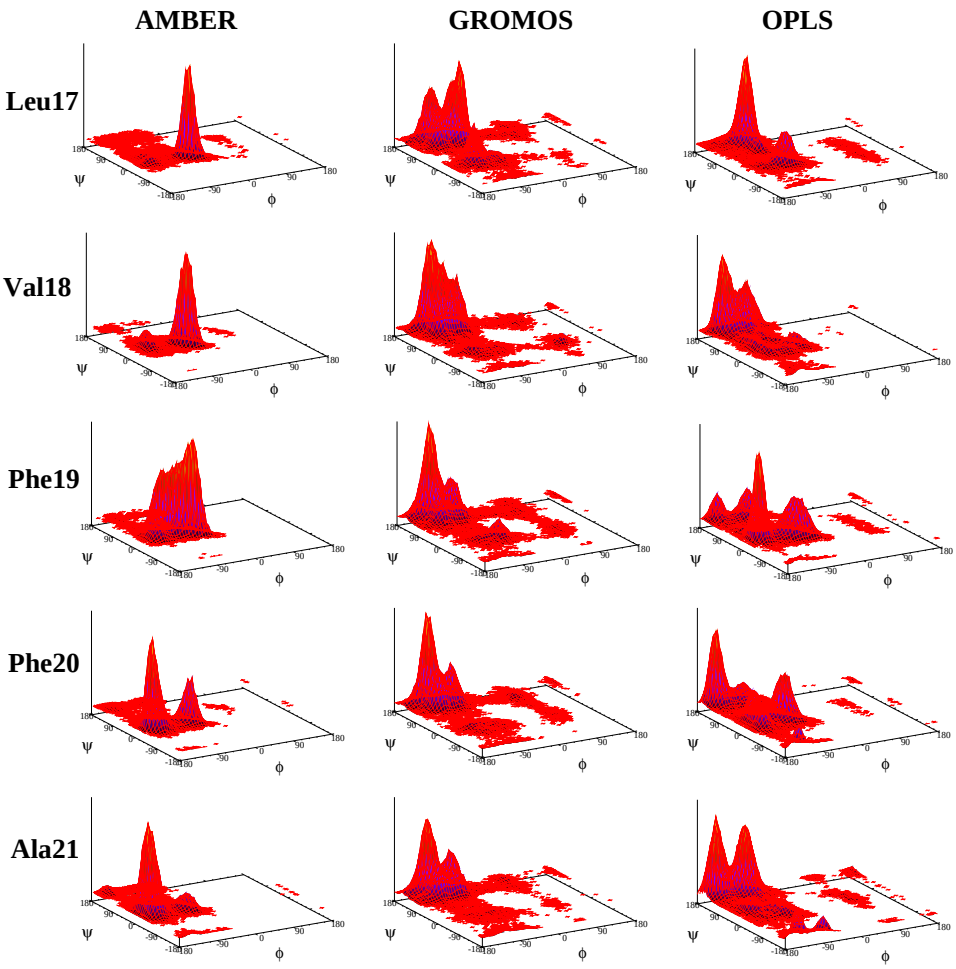

FIG. S1: Ramachandran ϕ, ψ probability distributions of residues of $A\beta_3$ in water as obtained from REMD simulations employing various force fields.

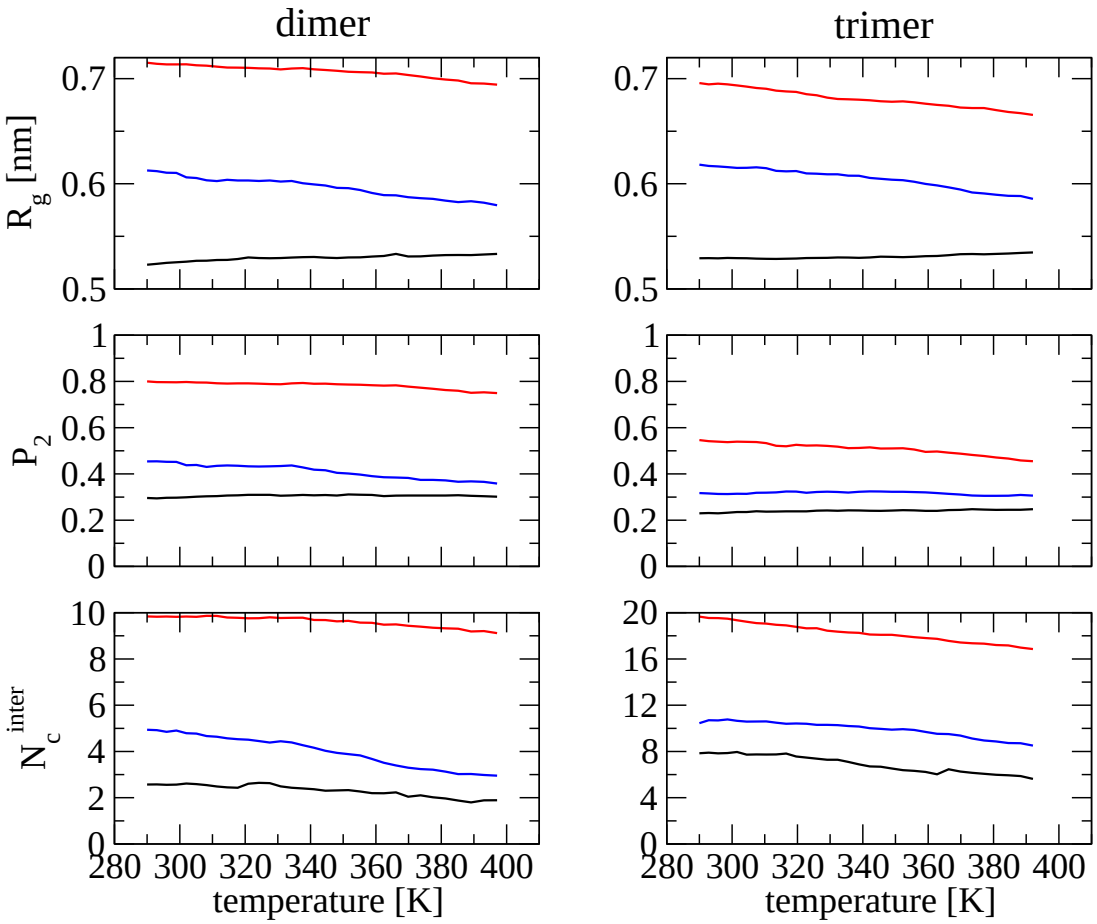

FIG. S2: The average values of the radius of gyration R_g, order parameter P_2 and the total inter-peptide contacts N_c^{inter} of Aβ_2 (left panels) and $A\beta_3$ (right panels) plotted as functions of temperature. Shown are results obtained from 50 ns REMD simulations employing various force fields AMBER (black), GROMOS (red) and OPLS (blue).

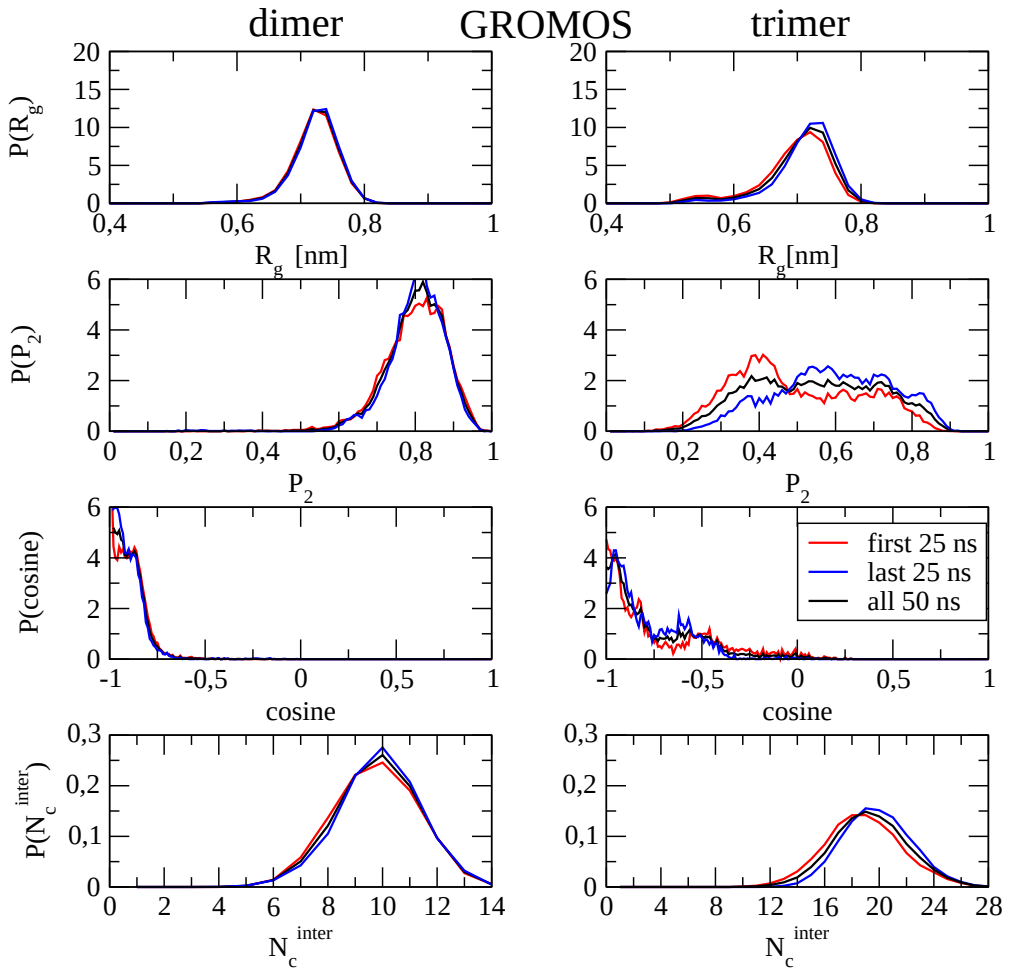

FIG. S3: Normalized distribution of the radius of gyration R_g, the order parameter P_2, the cosine of the angle between the end-to-end vectors of two peptides referred to as c(ij) for the dimer and the conditional probability for the trimer, and the total inter-peptide contacts N_c^{inter}. Shown are results obtained by GROMOS , using the first half (red), last half (blue) and the whole trajectory (black).

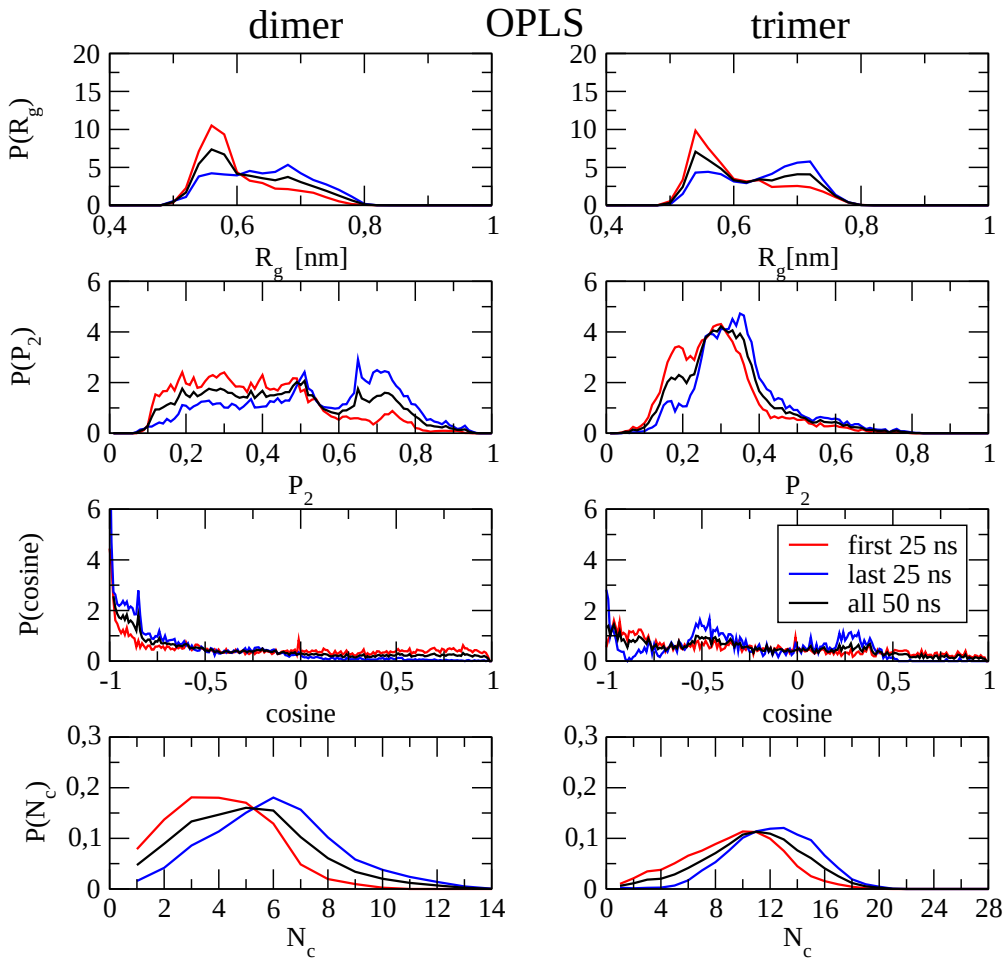

FIG. S4: Normalized distribution of the radius of gyration R_g, the order parameter P_2, the cosine of the angle between the end-to-end vectors of two peptides referred to as c(ij) for the dimer and the conditional probability for the trimer, and the total inter-peptide contacts N_c^{inter}. Shown are results obtained by OPLS, using the first half (red), last half (blue) and the whole trajectory (black).

FF	S	P	N_c^{intra}	ϕ_2, ψ_2	ϕ_3, ψ_3	ϕ_4, ψ_4	ϕ_5, ψ_5	ϕ_6, ψ_6	β	α	Coil
	1	52	10	-56,-32	-57,-15	-103, -3	-147,-14	-140, 1	0	2	98
	2	16	9	-126, -7	-57,-20	-89, -7	-140,-16	-135, 5	0	3	97
AMBER	3	11	8	-130,-11	-128, 50	-57,-27	-68,-12	-129, -9	5	23	73
	4	11	9	-59,-29	-131, 16	-59,-25	-64,-16	-128, -8	0	6	94
	5	10	10	-54,-32	-74,-11	-120,-15	-83,-14	-129, -5	0	7	93
	1	18	3	-85,118	-97,-39	-102,126	-112,127	-90,123	24	0	76
	2	17	3	-86,121	-98,117	-106,128	-111,132	-83,124	3	0	97
	3	16	10	-101,113	-24,110	65,-43	-80,-49	-122,102	12	1	87
GROMOS	4	14	4	-89, 97	-95,121	-95,-33	-99,-15	-97,125	9	0	91
	5	12	7	-101,138	-55,125	70,-35	-100,123	-48,104	0	0	100
	6	10	8	-82,-60	-125,118	-9,-63	-77,-41	-98,129	1	13	86
	7	7	3	-87,123	-100,124	-73,-18	-113,132	-87,122	2	0	98
	8	7	6	-104,-55	-107,-43	-103,141	-78,-42	-100,110	1	1	98
	1	28	5	-95,-13	-91,146	-132, -6	-126, 5	-131,165	0	3	97
	2	16	5	-95,109	-123,137	-137, -7	-140, -5	-127,166	1	0	99
	3	16	4	-82,136	-82, -4	-102, 7	-110,147	-86,135	34	4	62
OPLS	4	13	5	-93,-28	-108, 99	-88, 14	-105, -9	-127,116	1	6	93
	5	12	6	-89,114	-101, -9	-80, 2	-112, -5	-111, 93	1	26	73
	6	8	3	-87,128	-112,133	-126, -8	-137,164	-78,135	0	0	100
	7	7	6	-135,-30	-108,-17	-105,147	-91,-10	-106,147	0	1	99

TABLE S1: Characterization of the conformational states (S) indicated on the free energy landscapes shown in Fig.3 of Aβ_1. Shown are the population P (in %), the mean number of the total intra-peptide contacts N_c^{intra}, and secondary structure contents (in %).

FF	S	P	P_2	N_c^{intra}	N_c^{inter}	$c(12)$	α-helix	3_{10}-helix	π-helix	extended	bridge	turn	coil
	1	54	0.29	10	3	-0.23	7	28	0	0	0	20	45
AMBER	2	20	0.30	9	2	-0.03	3	18	0	0	0	40	38
	3	18	0.31	9	3	-0.31	4	18	0	0	0	43	34
	4	7	0.29	8	2	0.05	1	10	0	0	0	65	24
	1	50	0.80	2	10	-0.89	0	0	0	50	1	3	46
	2	25	0.84	2	10	-0.96	0	0	0	52	0	1	47
GROMOS	3	11	0.75	2	10	-0.87	0	0	0	36	1	5	57
	4	9	0.78	2	10	-0.89	0	0	0	37	1	6	57
	5	5	0.68	3	9	-0.89	0	0	0	35	5	6	53
	1	16	0.41	5	4	-0.38	0	1	0	1	3	40	53
	2	12	0.53	4	5	-0.61	0	0	0	17	3	22	58
	3	11	0.56	4	5	-0.60	0	1	0	8	3	23	61
	4	9	0.27	5	3	0.13	0	0	0	0	3	55	38
	5	9	0.48	3	6	-0.73	0	0	0	4	10	22	63
OPLS	6	9	0.49	4	5	-0.60	0	1	0	0	6	38	53
	7	8	0.41	3	5	-0.25	0	0	0	1	8	32	59
	8	7	0.38	2	6	-0.39	0	0	0	18	2	8	72
	9	6	0.31	6	3	-0.17	0	2	0	0	1	58	39
	10	6	0.70	2	9	-0.75	0	0	0	36	2	8	53
	11	5	0.58	3	5	-0.64	0	0	0	6	6	24	63
	12	3	0.21	4	3	0.19	0	0	0	0	1	34	65

TABLE S2: Characterization of the conformational states (S) indicated on the free energy landscapes shown in Fig.3 of Aβ_2. Shown are the population P (in %), the mean values of the order parameter P_2, the total intra-peptide contacts N_c^{intra}, the total inter-peptide contacts N_c^{inter}, the cosine of the angle between the end-to-end vectors of two peptides c(12) and the secondary structure contents (in %).

FF	S	P	P_2	N_c^{intra}	N_c^{inter}	c(12)	c(13)	c(23)	α-helix	3_{10}-helix	π-helix	extended	bridge	turn	coil
	1	51	0.24	10	8	-0.20	-0.13	-0.14	3	28	0	0	0	24	44
AMBER	2	22	0.23	9	7	-0.27	-0.06	-0.03	3	20	0	0	0	42	35
	3	19	0.24	9	8	-0.02	-0.15	-0.14	3	23	0	0	0	34	39
	4	7	0.22	8	8	-0.08	-0.10	-0.15	1	18	0	0	0	46	35
	1	32	0.56	2	20	-0.53	-0.48	-0.16	0	0	0	38	3	6	52
	2	15	0.54	2	19	-0.36	-0.56	-0.22	0	0	0	35	3	9	53
	3	12	0.54	2	19	-0.51	-0.48	-0.18	0	0	0	31	5	8	56
	4	11	0.45	3	18	-0.52	-0.14	-0.49	0	0	0	21	7	14	57
GROMOS	5	11	0.62	2	20	-0.37	-0.06	-0.57	0	0	0	24	2	10	63
	6	7	0.52	3	19	0.01	-0.10	-0.84	0	0	0	25	8	15	51
	7	5	0.49	3	18	-0.38	-0.77	0.24	0	0	0	16	8	18	58
	8	3	0.50	4	19	-0.82	0.33	-0.51	0	0	0	24	2	23	52
	9	3	0.56	2	22	-0.52	0.50	-0.81	0	0	0	38	1	9	52
	1	14	0.22	6	7	-0.25	0.10	-0.01	0	2	0	0	3	59	36
	2	12	0.31	3	11	-0.23	-0.47	-0.48	0	0	0	3	7	23	68
	3	9	0.36	3	13	-0.14	-0.40	-0.54	0	0	0	7	10	18	65
	4	9	0.26	4	10	-0.38	-0.50	-0.37	0	0	0	7	7	29	57
	5	8	0.28	4	9	-0.14	-0.44	-0.23	0	0	0	3	4	38	55
OPLS	6	8	0.35	2	13	-0.13	-0.12	-0.66	0	0	0	17	4	6	74
	7	8	0.40	3	13	0.09	-0.15	-0.83	0	0	0	33	1	24	42
	8	8	0.31	5	10	-0.46	-0.15	-0.15	0	1	0	1	2	42	53
	9	7	0.44	3	13	0.15	-0.74	-0.27	0	0	0	21	6	14	60
	10	7	0.31	4	10	-0.30	-0.29	-0.30	0	1	0	1	6	30	63
	11	6	0.36	3	13	-0.28	-0.36	-0.41	0	0	0	13	6	15	66
	12	4	0.22	5	8	-0.31	0.23	-0.03	0	1	0	0	1	56	42

TABLE S3: Characterization of the conformational states (S) indicated on the free energy landscapes shown in Fig.3 of $A\beta_3$. Shown are the population P (in %), the mean values of the order parameter P_2, the total intra-peptide contacts N_c^{intra}, the total inter-peptide contacts N_c^{inter}, the cosine of the angles between the end-to-end vectors of the ist and jnd peptides c(ij) ($i, j = 1, 2, 3$), and the secondary structure contents (in %).

System	FF	3_{10}-helix		extended		Turn		Coil	
		300 K	400 K	300 K	400 K	300 K	400 K	300 K	400 K
	AMBER	23	19	0	0	31	36	39	39
Aβ_2	GROMOS	0	0	47	32	4	10	48	55
	OPLS	0	0	7	1	31	43	55	51
	AMBER	24	20	0	0	31	36	40	39
$A\beta_3$	GROMOS	0	0	31	17	10	19	55	58
	OPLS	0	0	8	2	30	43	56	51

TABLE S4: Secondary structure contents (in %) of Aβ_2 and $A\beta_3$ at two temperatures 300 and 400 K. Shown are results using AMBER, GROMOS and OPLS force fields.