Effects of All-atom Force Fields on Amyloid Peptide Assembly: the Case of Aβ_{16-22} Dimer (Supporting Material)

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Table S1: **The characterizations of the disodered state (*DS*), intermediate state (*IS*) and fibril states (*FS*).** Here, $P-FS$ and $AP-FS$ mean parallel fibril-like state and antiparallel fibril-like, respectively. The *CP* indicates conformational population (in %) of a state, while *RP* is number of MD runs in which the state waas observed. *IRS* and *ORS* are labels for in-register and out-of-register antiparallel β-sheet structures, respectively. The data was calculated from whole 200 ns of simulation time and all one hundred MD runs for each force field.

FFs	*DS*	*IS*	*FS*									
	CP	*CP*	*CP*	τ (ns)	*RP*	CP_{AP-FS}/CP_{P-FS}	RP_{AP-FS}	RP_{P-FS}	CP_{IRS}	RP_{IRS}	CP_{ORS}	RP_{ORS}
A94	99.3	0.6	0.1		6	100/0	6	0	0.0	6	0.0	4
A96	15.2	14.3	70.5	16 ± 1.9	100	98/2	100	11	35.6	95	34.9	81
A99	98.5	1.0	0.5		9	89/11	8	1	0.0	7	0.0	6
A99SBi	39.2	19.2	41.6	33 ± 4.4	95	95/5	93	5	19.2	76	19.5	74
A03	50.9	23.5	25.7	26 ± 3.8	90	100/0	90	6	11.8	86	11.3	78
A12SB	86.0	6.6	7.4		42	100/0	42	0	1.2	28	1.9	35
A14SB	34.5	12.8	52.6	25 ± 3.4	97	99/1	96	2	28.5	92	22.0	75
C22	42.9	30.3	26.8	35 ± 3.9	95	97/3	95	4	13.0	70	12.4	74
C36	49.7	20.9	29.4	50 ± 5.2	92	100/0	92	5	11.8	59	15.2	62
C36m	48.1	23.2	28.7	44 ± 4.6	95	97/3	95	6	10.4	59	16.9	76
OPLS	32.1	22.9	45.1	25 ± 4.1	94	100/0	94	0	21.4	77	21.0	67
G43a1	11.1	43.1	45.8	5 ± 1.1	100	100/0	100	19	21.0	98	24.8	97
G43a2	12.0	39.8	48.2	4 ± 1.1	99	100/0	99	38	20.6	97	27.2	98
G45a3	5.3	32.0	62.7	2 ± 0.3	100	100/0	100	25	36.4	100	26.3	83
G53a5	16.3	26.7	57.0	11 ± 1.8	100	100/0	100	28	24.1	96	32.9	90
G53a6	5.8	29.4	64.8	7 ± 1.7	100	100/0	100	11	34.1	91	30.7	71
G54a7	17.1	49.7	33.2	12 ± 2.3	99	100/0	99	5	15.1	97	17.7	73

Table S2: **The statistics of the ten dineric antiparallel β-sheet structures types (see figure 5 in main text).** The *CP* indicates conformational population (in %) of a state, while *RP* is number of MD runs in which the state waas observed. The data was calculated from whole 200 ns of simulation time and all one hundred MD runs for each force field.

FFs	(I)		(II)		(III)		(IV)		(V)		(VI)		(VII)		(VIII)		(IX)		(X)	
	CP	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*	*CP*	*RP*
A94	0.0	5	0.0	0	0.0	0	0.0	1	0.0	0	0.0	0	0.0	2	0.0	0	0.0	2	0.0	0
A96	23.0	62	1.0	5	0.0	2	12.6	75	0.8	5	3.7	15	14.5	47	0.0	1	14.7	34	0.1	5
A99	0.0	4	0.0	0	0.0	0	0.0	5	0.0	1	0.0	0	0.0	6	0.0	0	0.0	0	0.0	0
A99SBi	7.5	38	0.5	8	0.0	3	11.6	62	0.0	0	5.1	16	5.4	33	0.0	1	8.4	37	0.0	2
A03	4.8	57	0.0	10	0.0	0	7.0	78	0.2	7	0.0	5	5.4	57	0.0	0	5.7	34	0.0	0
A12SB	1.1	18	0.0	2	0.0	2	0.1	23	0.0	0	0.4	8	0.1	12	0.0	0	1.2	23	0.0	1
A14SB	21.4	55	0.0	1	0.1	1	7.1	76	0.0	1	1.0	10	7.6	34	0.0	0	13.3	51	0.1	4
C22	8.9	46	0.1	8	0.1	3	4.0	37	0.1	3	2.4	13	1.5	30	0.0	3	8.3	45	0.0	1
C36	5.4	36	0.0	3	0.0	1	6.4	32	0.0	2	4.8	22	3.0	24	0.0	0	7.4	30	0.0	3
C36m	3.6	25	0.4	11	0.0	1	6.8	37	0.0	1	3.4	17	3.4	25	0.0	2	9.7	39	0.0	3
OPLS	15.1	47	0.0	3	0.3	3	6.3	46	0.0	2	3.5	11	2.4	14	0.0	0	14.7	46	0.0	2
G43a1	12.4	84	0.5	8	0.0	5	8.6	87	0.0	17	2.6	25	14.2	88	0.0	3	7.5	51	0.0	1
G43a2	15.4	89	1.1	14	0.2	5	5.2	84	0.1	31	0.8	19	19.7	90	0.0	1	5.3	51	0.0	1
G45a3	22.2	88	0.1	11	0.0	5	14.2	79	0.1	12	2.3	27	13.0	70	0.0	1	10.8	47	0.0	0
G53a5	16.9	67	2.1	8	0.2	3	7.2	71	0.2	16	1.9	21	14.7	69	0.1	6	13.7	50	0.0	2
G53a6	25.5	56	0.3	4	0.1	2	8.6	52	0.1	13	3.6	15	16.1	53	0.0	0	10.6	25	0.0	2
G54a7	10.4	78	0.3	8	0.1	4	4.7	68	0.0	16	2.7	14	5.0	49	0.0	3	9.7	41	0.0	1

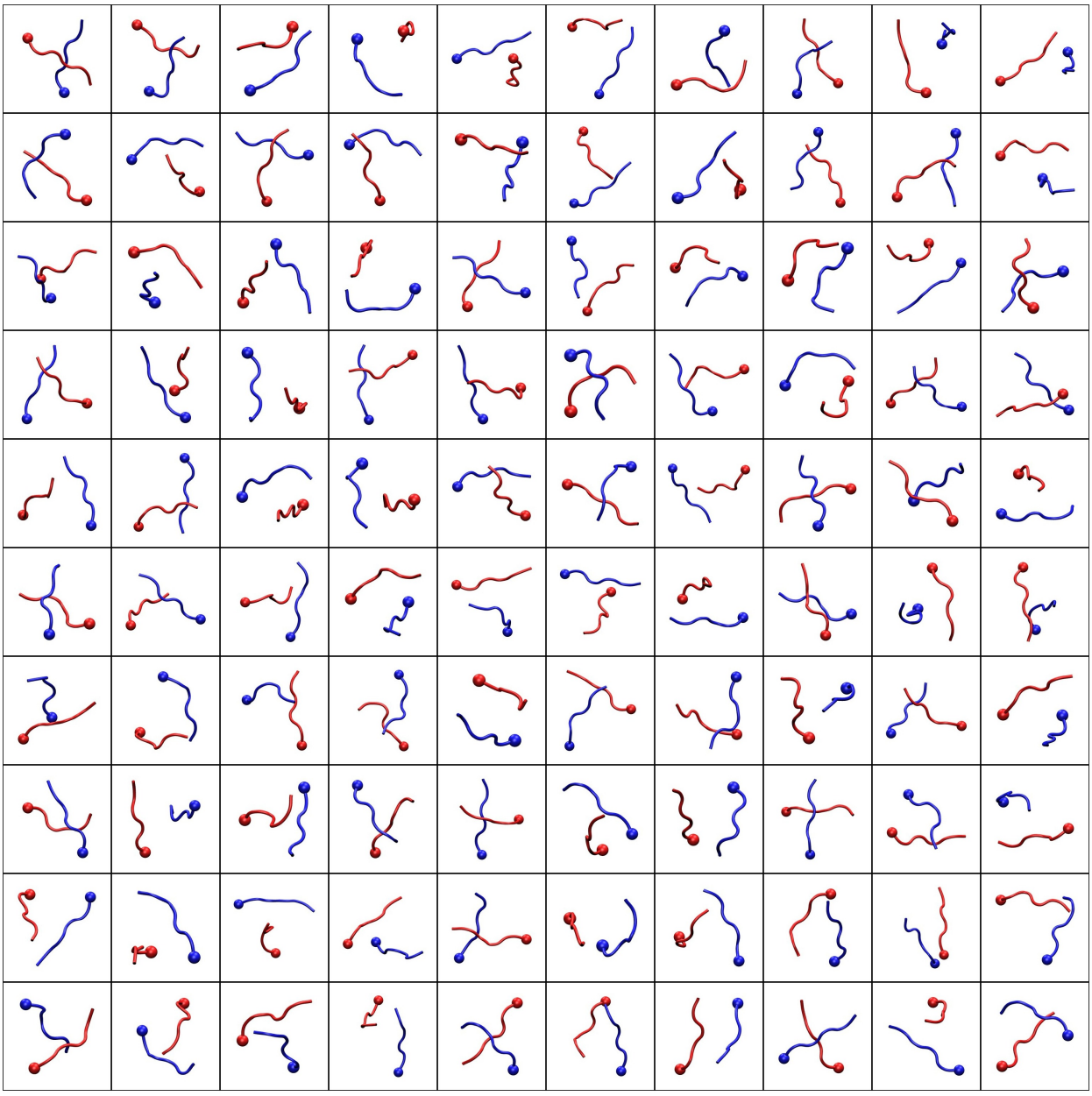

Figure S1: The 100 initial structures of the Aβ_{16-22} dimer are built by randomly rotating and placing two monomers (red and blue) in the space. The balls indicate the N-terminus of the peptides. The mean values of the distributions of the inter-chain distance, the cosine angle between two end-end vectors of two chains, and the order parameter P_2 of these 100 structures are 0.8 nm, 0° and 0.3, respectively.

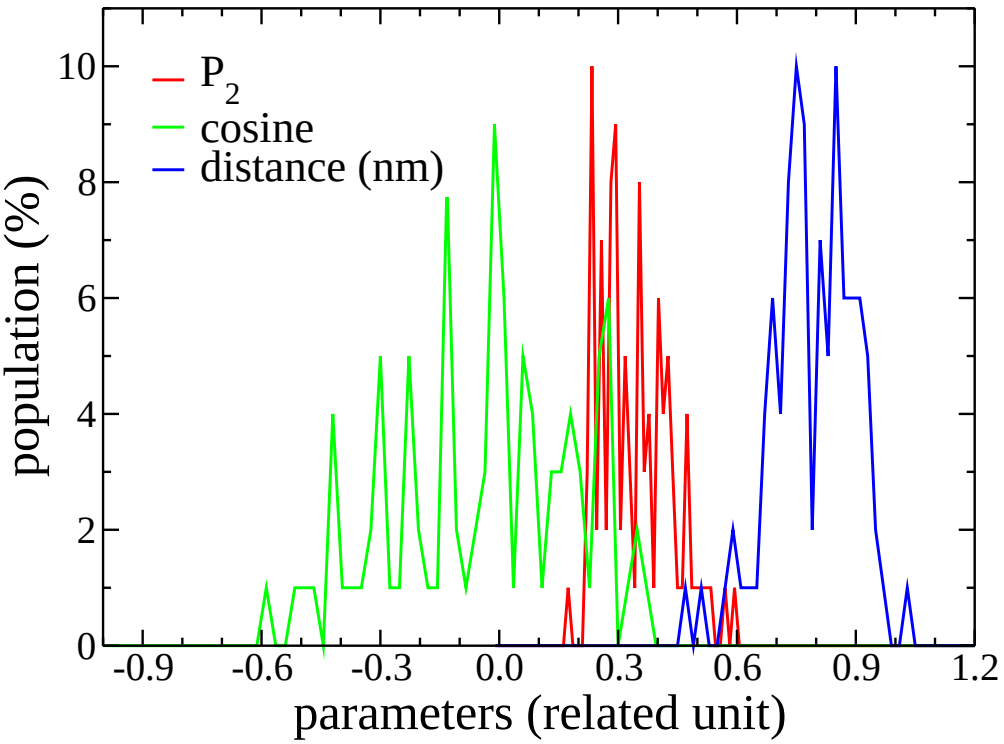

Figure S2: Distribution of the P_2 (red line), the cosine of the angle between the end-to-end vectors of two peptides (green line) and the distance (in nm) between the mass centers of two peptides (blue line) in the one hundred dimeric initial structures.

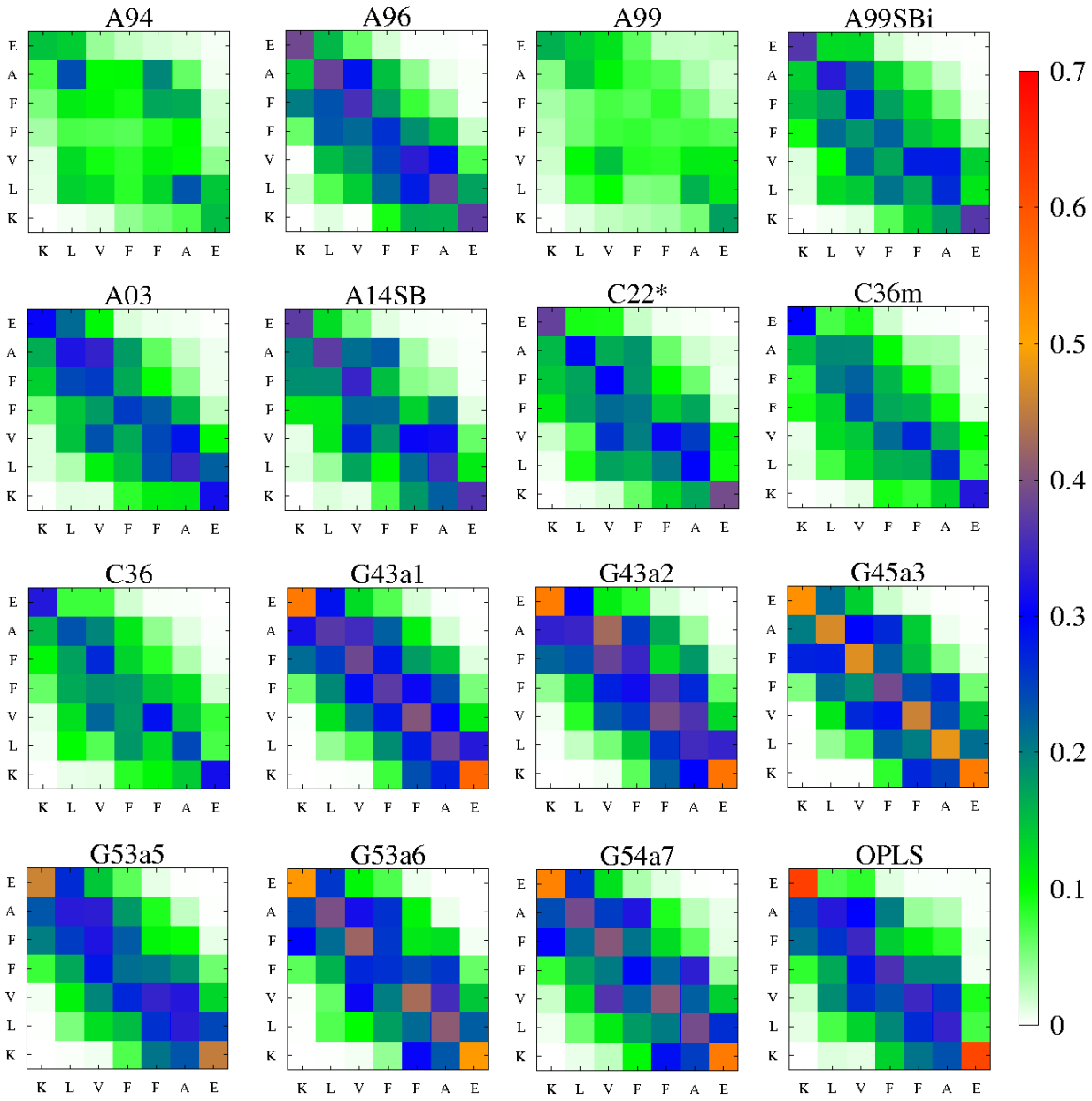

Figure S3: The intermolecular side chain-side chain contact maps. The data was calculated from the one hundred runs of 200-ns MD simulations for each force field.

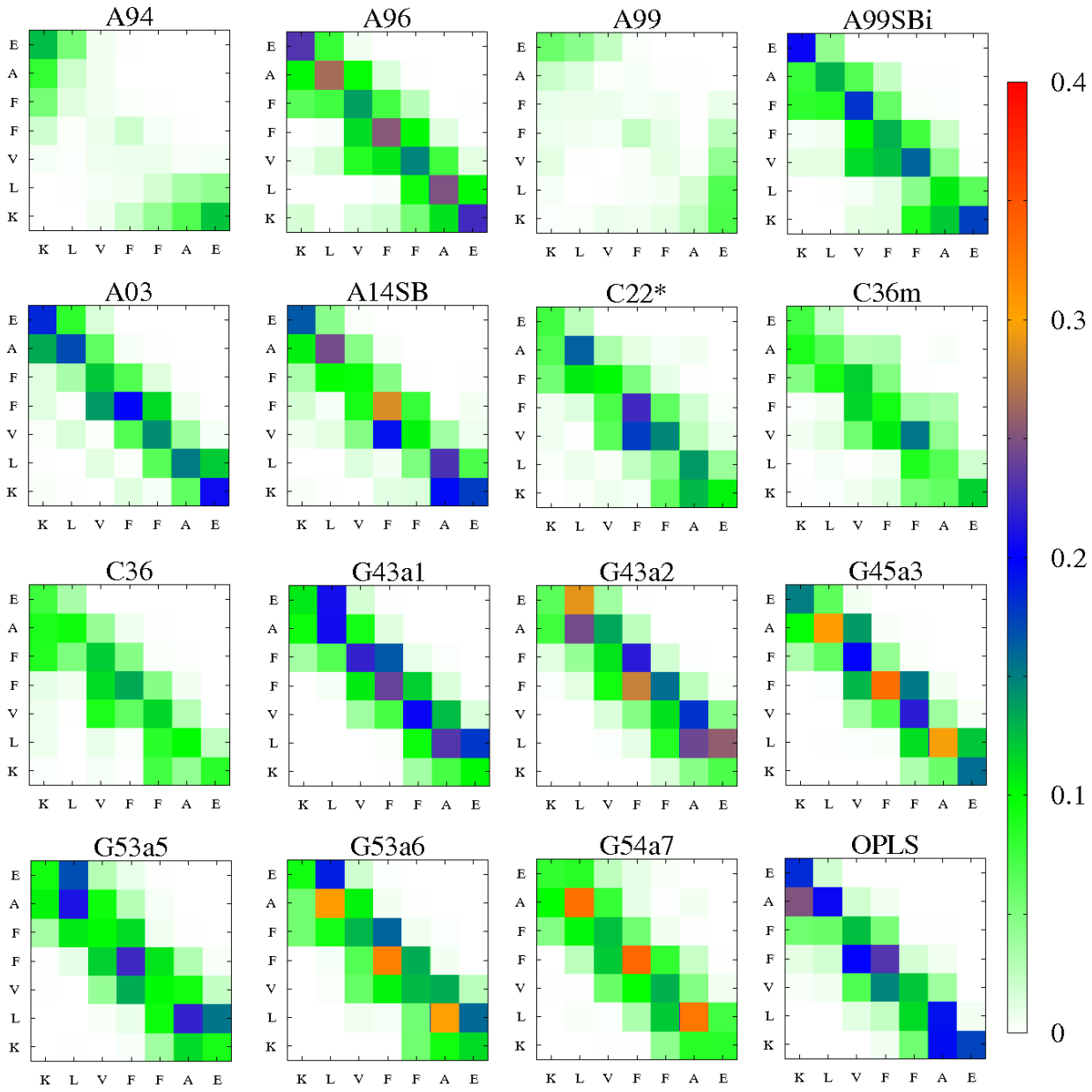

Figure S4: The intermolecular backbone hydrogen bond maps. The data was calculated from whole 200 ns of simulation time and all one hundred MD runs for each force field.

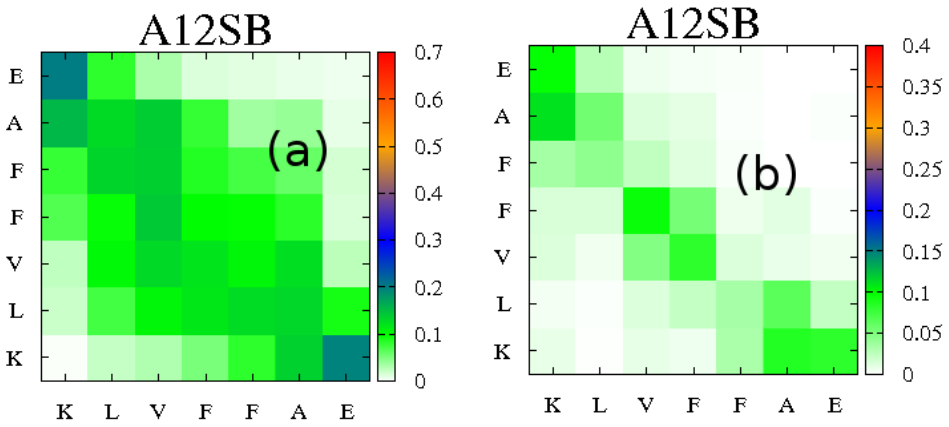

Figure S5: The intermolecular sidechain-sidechain contact and intermolecular backbone hydrogen bond maps of AMBER12SB force field. The data was calculated from whole 200 ns of simulation time and all one hundred MD runs.

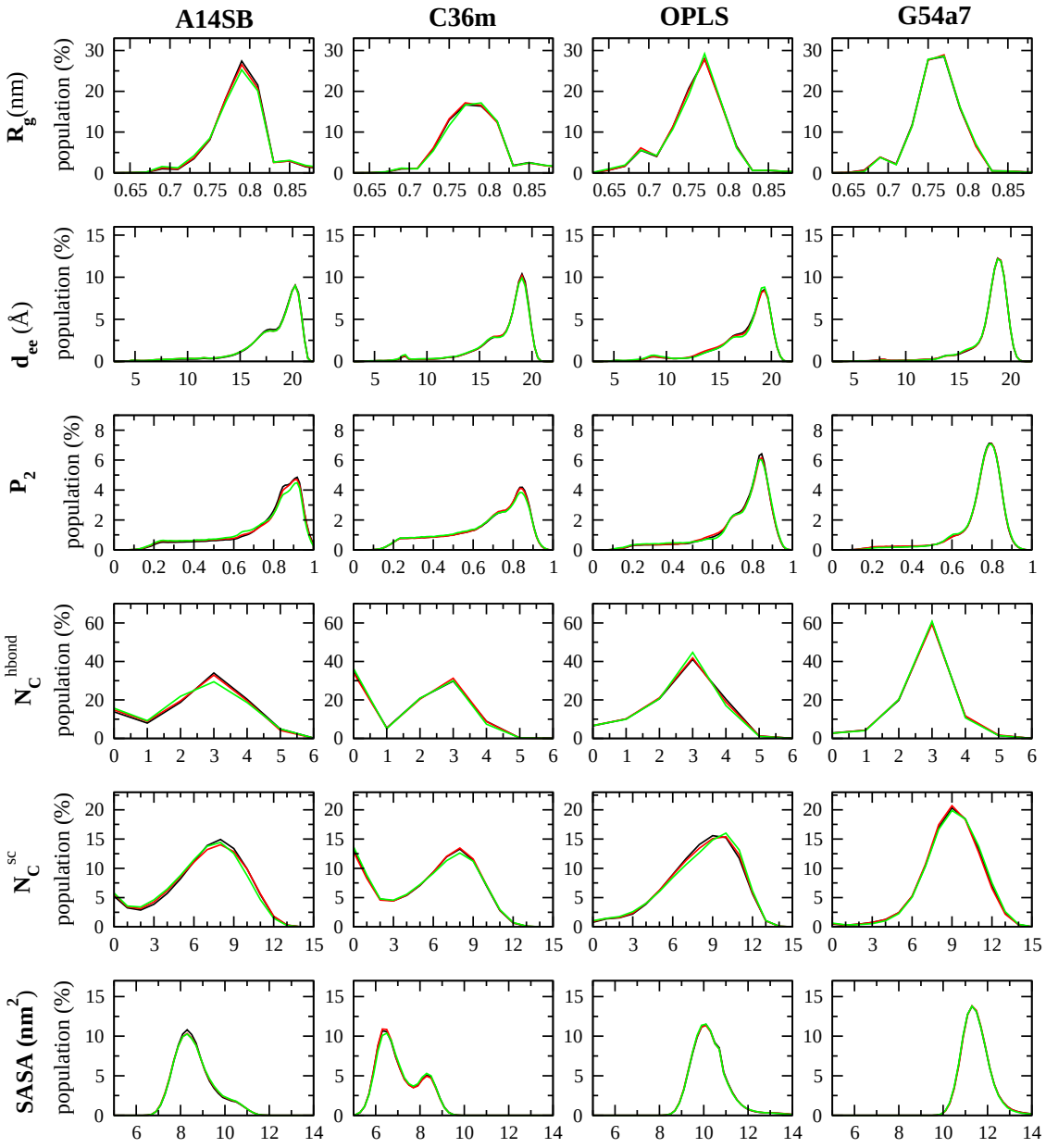

Figure S6: Normalized distributions of the radius of gyration (R_g), the end-to-end distance (d_{e2e}), the order parameter (P_2), the intermolecular backbone H-bonds (N_C^{hbond}), the intermolecular side chain-side chain contacts (N_C^{sc}) and the solvent accessible surface area (SASA). Shown are results obtained by A14SB, C36m, OPLS and G54a7 force fields and averaged over all conformations from 100 trajectories (black lines), random picked-up 75 trajectories (red lines) and random picked-up 50 trajectories (green lines). Excellent agreements are observed between results obtained using the three ensembles for all coordinates and all the four force-fields, as well as other rest force fields (data not shown).

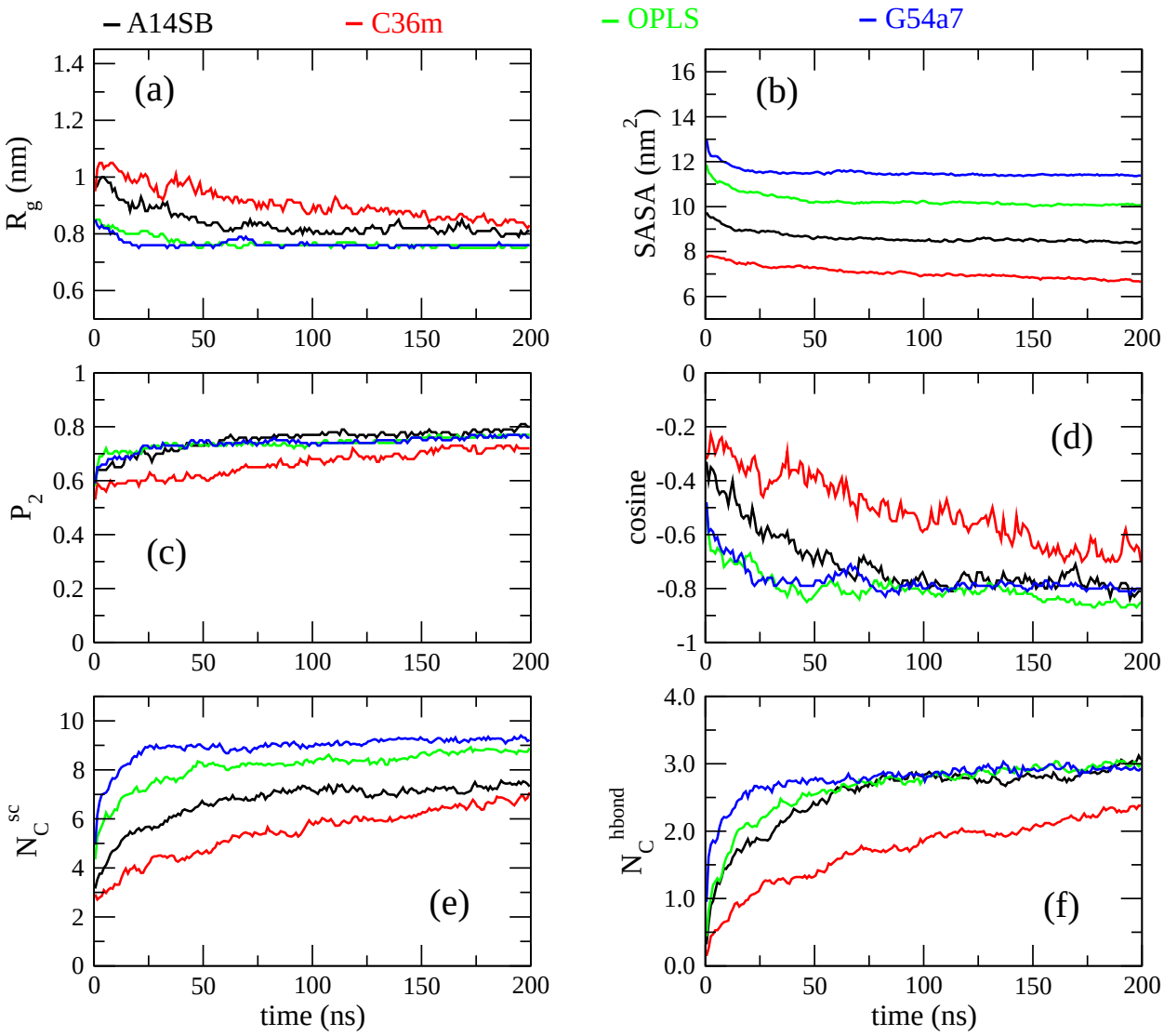

Figure S7: Time evolution of the recaction coordinates including R_g (a), SASA (b), P_2 (c), cosine (d), intermolecular side chain-side chain interaction (e) and intermolecular backbone H-bond (f) in A14SB, C36m, OPLS and G54a7 force fields. The data was averaged for every nanosecond and from the 100 trajectories for each force field. All quantities reach the plateau values after 100 ns, indicating that the system is well-equilibrated. The same well-equilibrated results are obtained for the rest other force fields (data not shown).

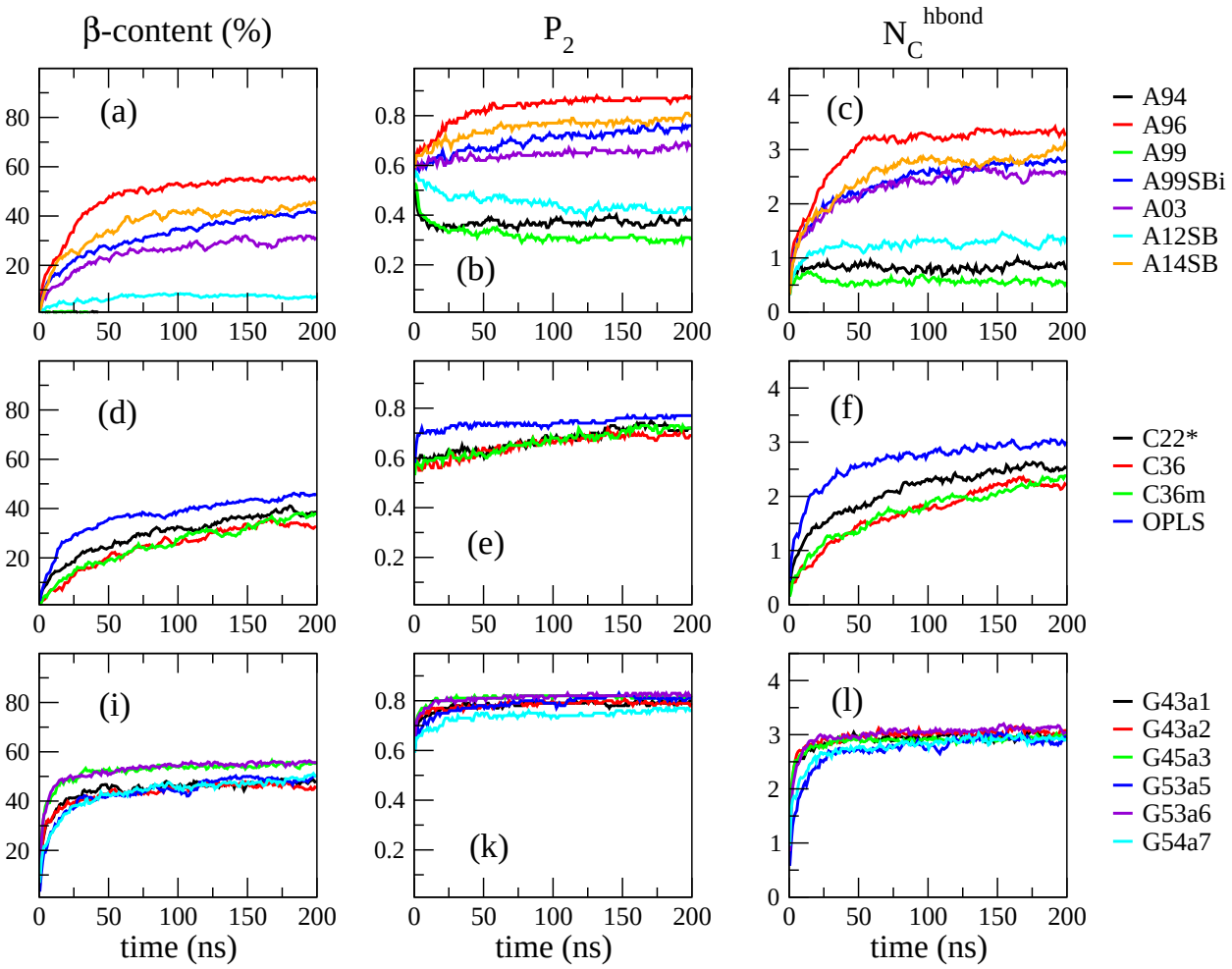

Figure S8: Time evolution of β content, P_2 and intermolecular backbond H-bond of the dimer in the 17 force fields. The data was averaged for every nanosecond and from the 100 trajectories for each force field.