SUPPORTING INFORMATION

Factors and atomistic parameters in the PACSAB force field equations

The multiplicative factor C of the implicit solvation term in equation 7 is $C=1/(2\pi^{(3/2)}\lambda)$, where we have chosen the correlation length λ = 3.5 A [24]. The solvation free energies ΔG_i of each atom are taken from the ΔG_{free} column of Table I of [24], and the volumes v_i are taken from the "Volume" column of the same table. Regarding the atomistic van der Waals term (first equation of Appendix B), ε^* is taken from the Table IV of [23] , and R^* is the r_{min} of the same table.

Table S1. PACSAB simulation speed (time simulated/CPU core time) for different systems

System	Number of particles	Speed (ns/h)
4 Aβ40 peptides (Aβ40 solution)	1152	5.5
α-synuclein	967	4.8
1FVQ protein	513	24
1PPE complex	1781	3.1

Table S2. Average RMSDs at the end of the simulations for several proteins used in the test sets of PaLaCe [5], PRIMO [7] and OPEP[12]. Our PACSAB simulations are 100 ns long for all the proteins.

PDB	RMSD (A) with PACSAB	CG model in the original work, length of the trajectory	RMSD (A) with the CG model of the original work
1TZV	5	PaLaCe, 100 ns	4.5
1MLC	3.4	PaLaCe, 100 ns	3
1TMY	5.5	PaLaCe, 100 ns	4.5
3GB1	4.2	PRIMO, 50 ns	2.6
1D3Z	4.4	PRIMO, 50 ns	3.3
1BTA	5	PRIMO, 50 ns	2.6
1FKS	4.5	PRIMO, 50 ns	3.0
1A2P	5.9	PRIMO, 50 ns	3.9
2AAS	6.2	PRIMO, 50 ns	4.4
1GYZ	6.1	OPEP, 30 ns	4.2
1FAF	5.8	OPEP, 30 ns	4.2
1FCL	4.2	OPEP, 30 ns	3
1B75	4.8	OPEP, 30 ns	5.3
2B86	3.5	OPEP, 30 ns	4.5
1AFP	5.1	OPEP, 30 ns	3.6

Table S3. Complexes of the test set. From left to right, experimental binding energies, number of residues of the receptor, number of residues of the ligand, RMSD respect to initial structure after a 1ns DMD trajectory when starting from the experimental complex structure, and the same when starting from the best scored false positive (see main text).

COMPLEX	ΔG (kcal/mol)	N_{res} (receptor)	N_{res} (ligand)	$RMSD_{exp}$ (Å)	$RMSD_{fp}$ (Å)
1AY7	-13.2	96	89	5.6	17.6
1BUH	-10.1	287	70	33.4	10.1
1BVN	-10.5	496	71	6.5	41.3
1E6J	-10.3	218	209	13.2	30.6
1FSK	-13.1	220	159	14.9	34.1
1GPW	-11.3	253	200	5.4	37.2
1IQD	-15	200	155	7.8	30.9
1M10	-11.2	199	267	8.7	37.4
1MAH	-14.5	533	61	5.5	8.6
1OPH	-11.3	375	223	7.8	16.9
1PPE	-15.6	223	29	4.0	14.3
1R0R	-14.2	274	51	3.9	6.4
2B42	-12.1	364	184	6.6	13.8
2HLE	-10.1	188	133	6.2	29.9
2HQS	-10.2	412	108	55.0	24.9
2HRK	-11.0	177	105	14.5	45.0
2I25	-12.3	114	129	7.0	32.5
2JEL	-11.6	218	85	34.8	38.0
2SIC	-13.8	275	107	6.0	44.3
2SNI	-16.0	275	64	3.7	6.2

Figure S1. DSSP plot for secondary structure transitions in the PACSAB trajectory of a Aβ40 peptide. The simulation started from a completely extended random coil conformation.

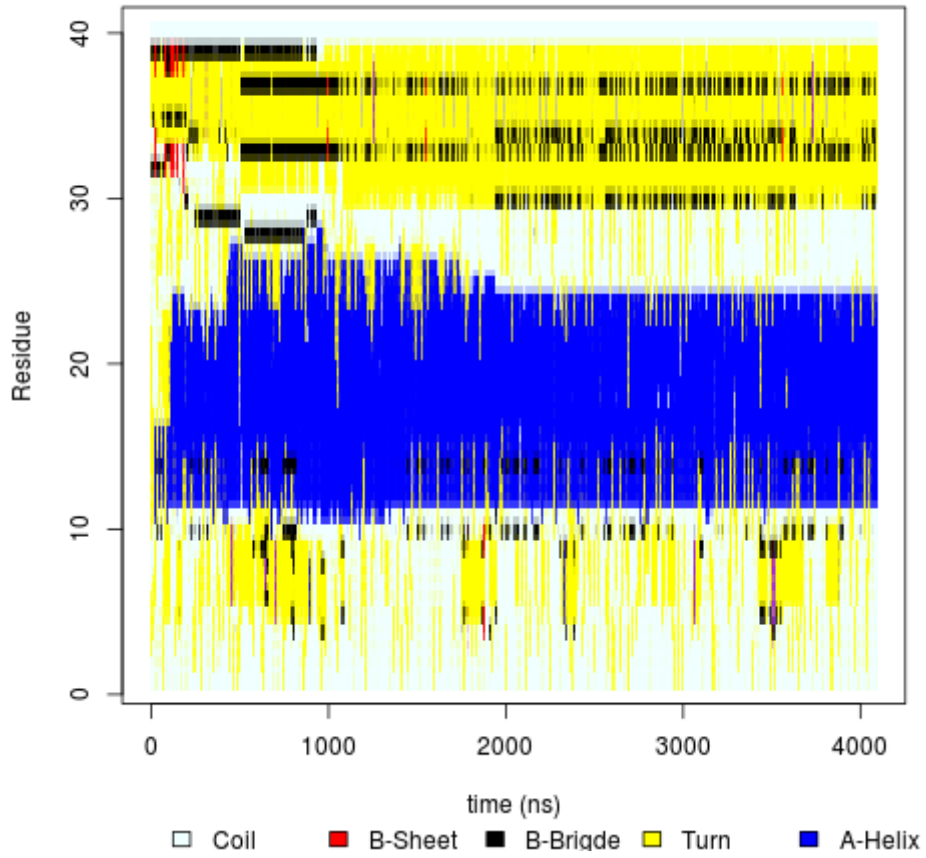

Figure S2. Secondary structure probabilities obtained with PACSAB for the Aβ40 peptide along sequence. Solid lines correspond to the simulation of a single Aβ40 peptide, and dashed lines to the simulation of the Aβ40 solution, where oligomers are formed. α-helix probability in black and β-strand probability in red.

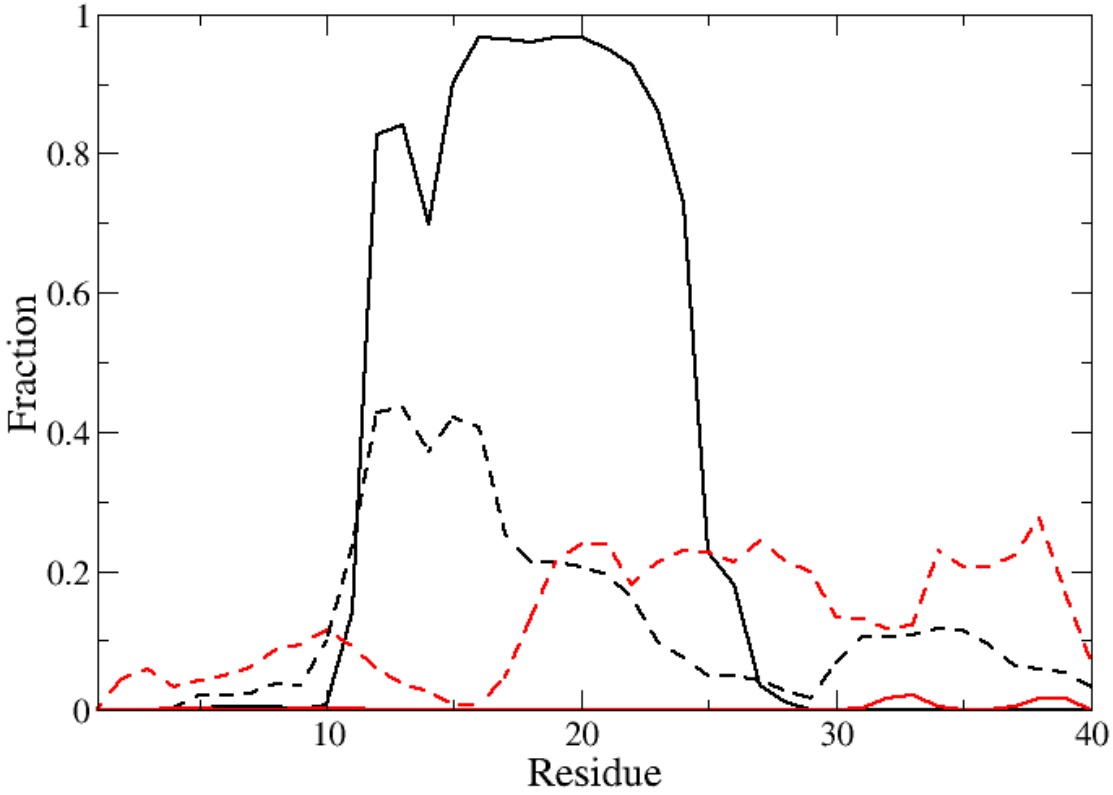

Figure S3. Intermolecular contact maps in Aβ40 dimers. Blue corresponds to zero contacts, red to many contacts.

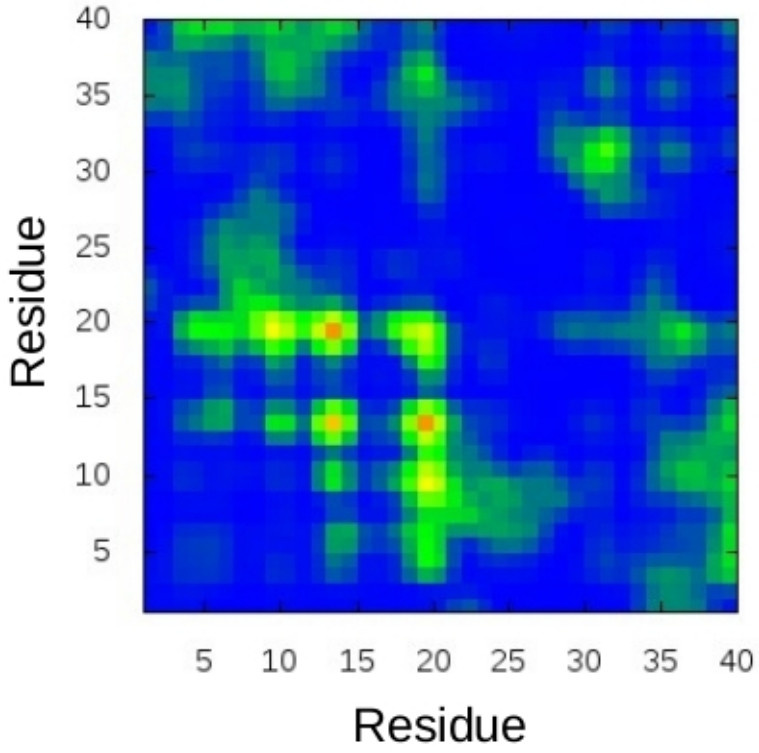

Figure S4. Intramolecular contact maps for an isolated Aβ40 peptide (left) and Aβ40 dimers (right). Blue corresponds to zero contacts, red to many contacts.

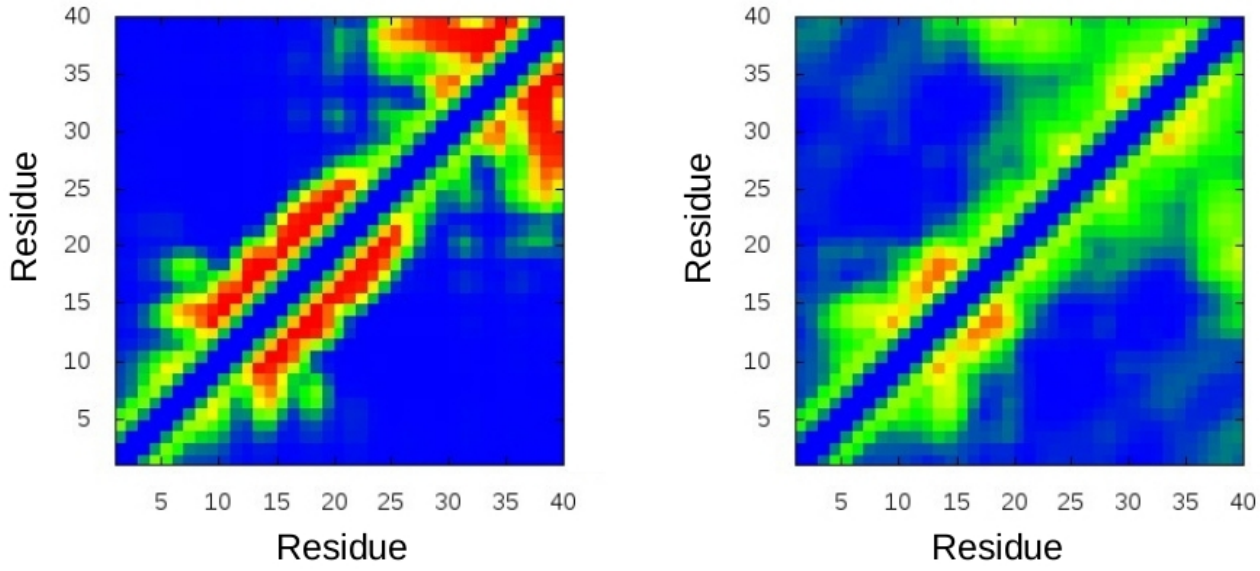

Figure S5. Folding of a three strand β-sheet (top) and of the α-helix EK peptide (below). At left, the superposition of the structure at the end of the simulation (cyan) and the experimental structure (orange). At right, the RMSD respect to the native conformation along the simulation. The β-sheet is the Gly5-Trp29 segment of the protein 1I6C. The sequence of the EK peptide is AEAAKAAEAAKA.

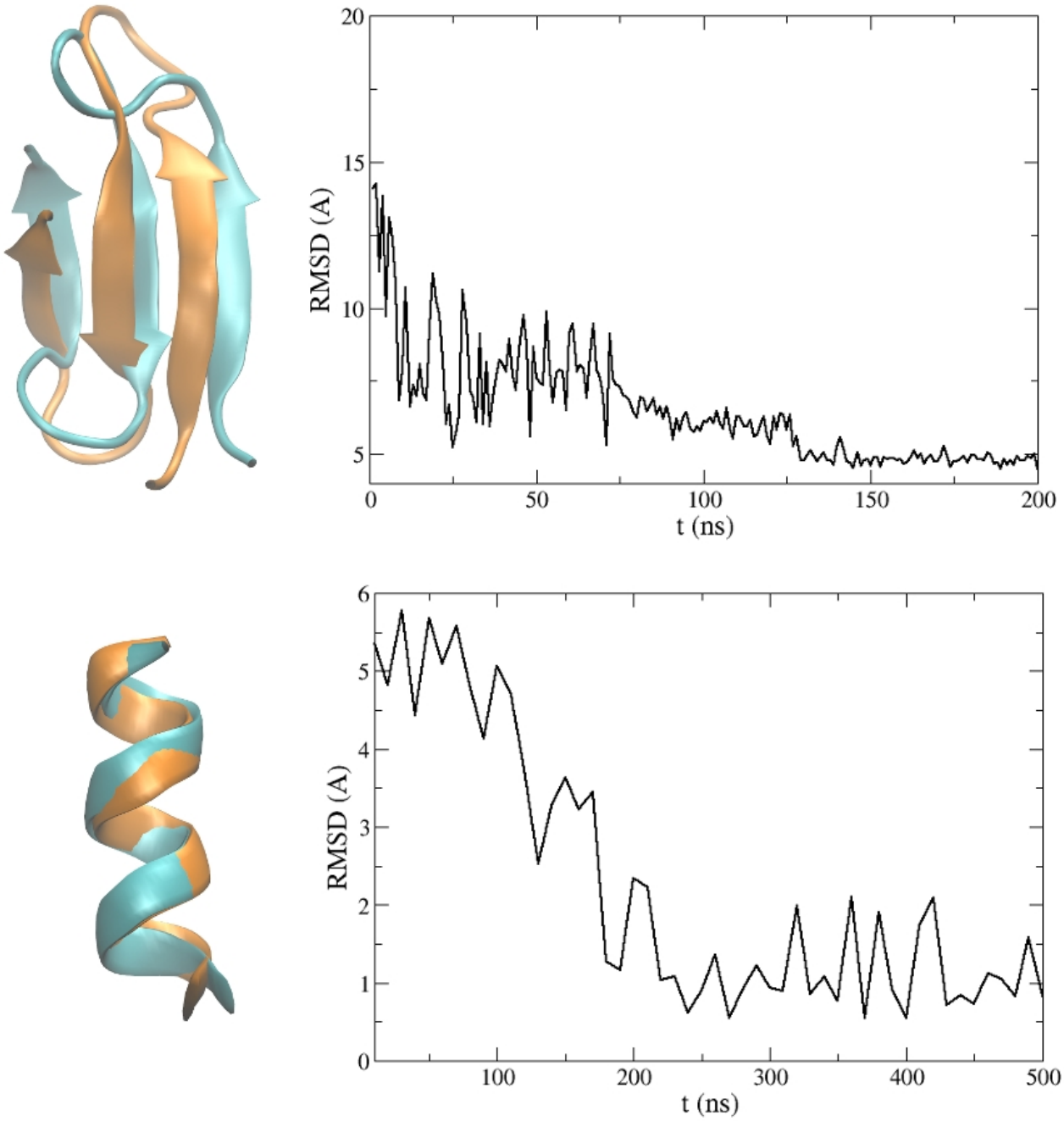

Figure S6. Ramachandran plot of the protein benchmark that we have used. Crystal structures (left) and structures after 500 ns of simulation with PACSAB (right)

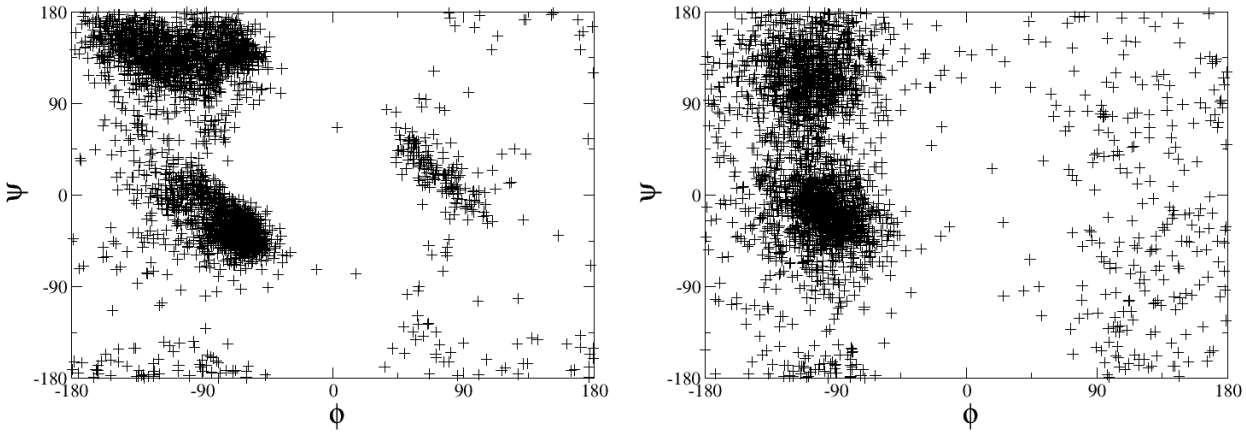

Figure S7. Contact maps of the proteins in the benchmark. Blue corresponds to zero contacts, red to many contacts. Above the diagonal, contact map of the crystal; below the diagonal, average of the contacts over the last 100 ns of trajectory

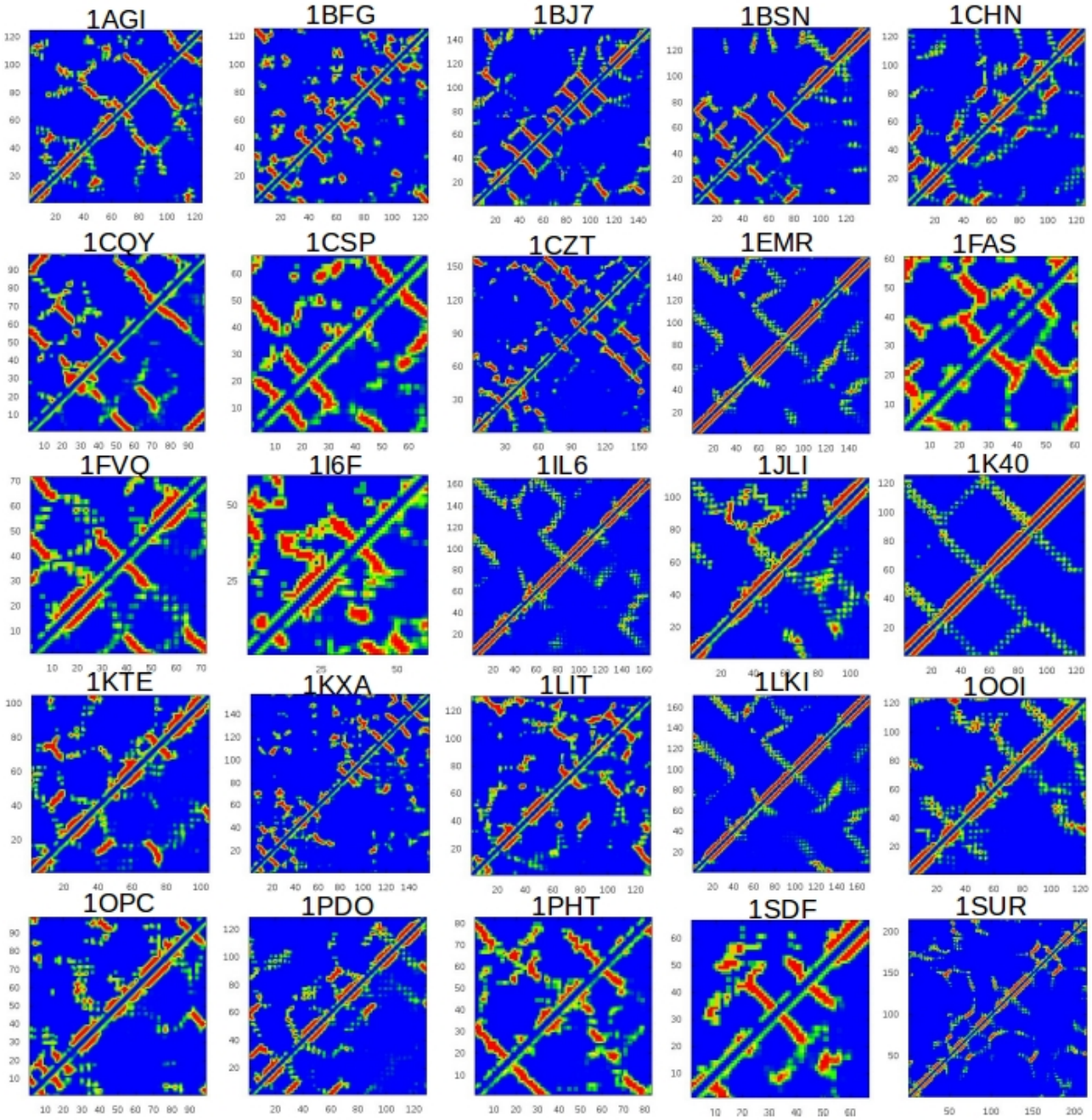

Figure S8. Structure of several proteins of the benchmark after 500 ns of simulation with PACSAB (cyan) compared to crystal structure (orange). Same ordering as in the contact maps figure.