Supporting Information to

"Cross Dimerization of Amyloid-β and αSynuclein Proteins in Aqueous Environment: a Molecular Dynamics Simulations Study"

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Table S1. Salt bridge distances

Cluster	Salt Bridge	d^{SB}
C1	K6 – D7	9.1 (2.9)
	K21 – E11	4.5 (2.7)
	E28 – R5	3.6 (0.5)
C2	K6 – D1	7.4 (4.3)
	K32 – D1	5.5 (3.4)
	K32 – E3	5.9 (1.9)
	K80 – D7	2.9 (0.2)
	K80 – E3	3.3 (0.3)
C3	K6 – E3	5.9 (2.4)
	K12 – E22	5.7 (3.2)
C5	K6 – E22	4.0 (1.3)
	K6 – D23	5.6 (2.2)
	K10 – D23	2.9 (0.3)
	K12 – D1	3.5 (0.6)
	E83 – K28	8.5 (3.4)

Mean value of the inter-residue sidechain distances (d^{SB}, in Å) between the residues that form salt bridges in the clusters a) C1, b) C2, c) C3, d) C5. Standard deviations are provided in braces. The first residue belongs to $\alpha Syn_{1\text{-}95}$; the second residue belongs to $A\beta_{1\text{-}42}$.

Table S2. Details of internal contacts and compactness of peptides in different clusters

Clusters	**<Nint.$^{A\beta}$>**	**<Nint.$^{\alpha S}$>**	**$R_g^{A\beta}$**	**R_g^{aS}**
C1	141.4 (7.4)	485.0 (18.0)	12.0 (0.5)	14.6 (0.2)
C2	141.5 (9.1)	414.6 (12.9)	14.67 (0.7)	16.7 (0.5)
C3	153.1 (7.6)	467.1 (12.9)	10.9 (0.2)	14.4 (0.2)
C4	126.0 (5.7)	361.9 (9.3)	14.2 (0.4)	23.8 (0.7)
C5	141.1 (7.8)	454.2 (13.2)	12.9 (0.3)	16.9 (0.3)

Mean values of the total number of internal contacts formed in the A$\beta_{1\text{-}42}$ ($N_{int}^{A\beta}$) and $\alpha Syn_{1\text{-}95}$ ($N_{int}^{\alpha S}$) proteins in the five clusters. The corresponding radii of gyration (in Å) have been denoted as $R_g^{A\beta}$ and $R_g^{\alpha S}$.

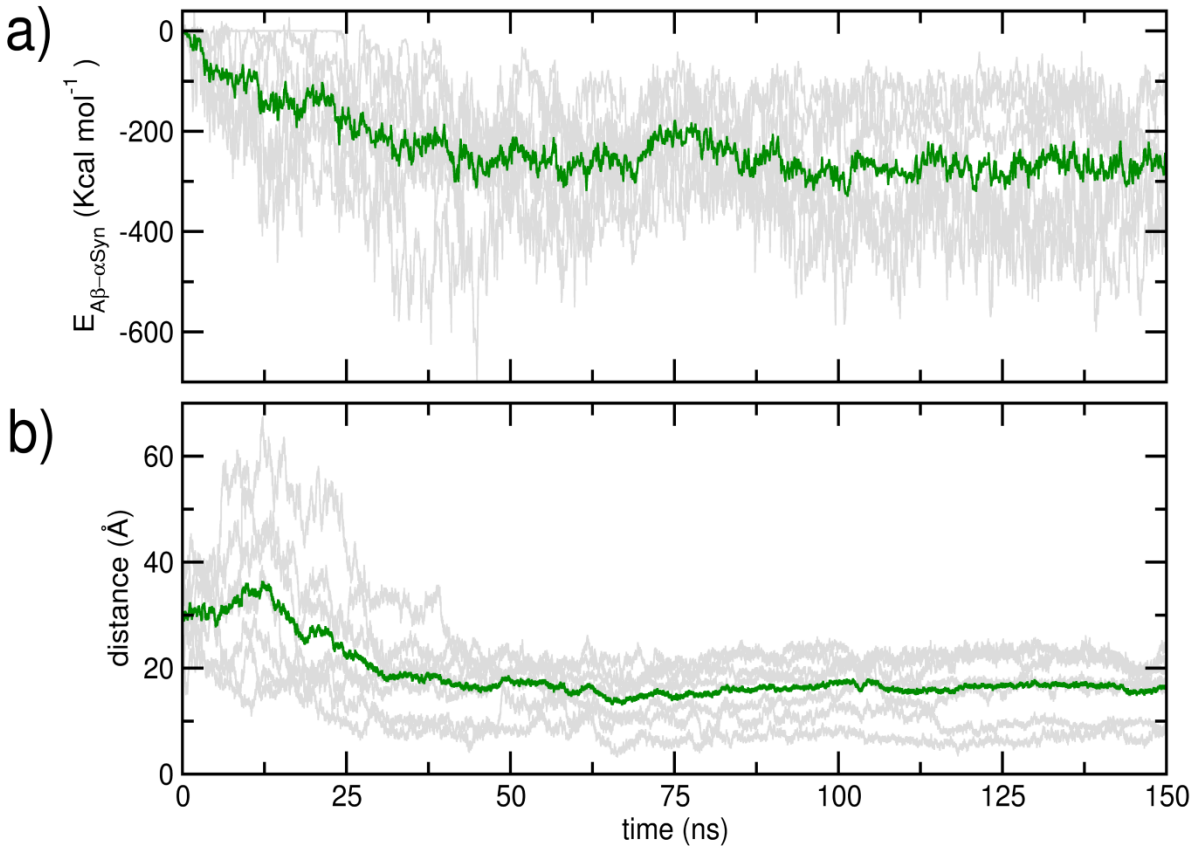

Figure S1. Evolution of the a) total inter-peptide interaction strength, and b) inter peptide distance over 150 ns for the dimerising trajectories.

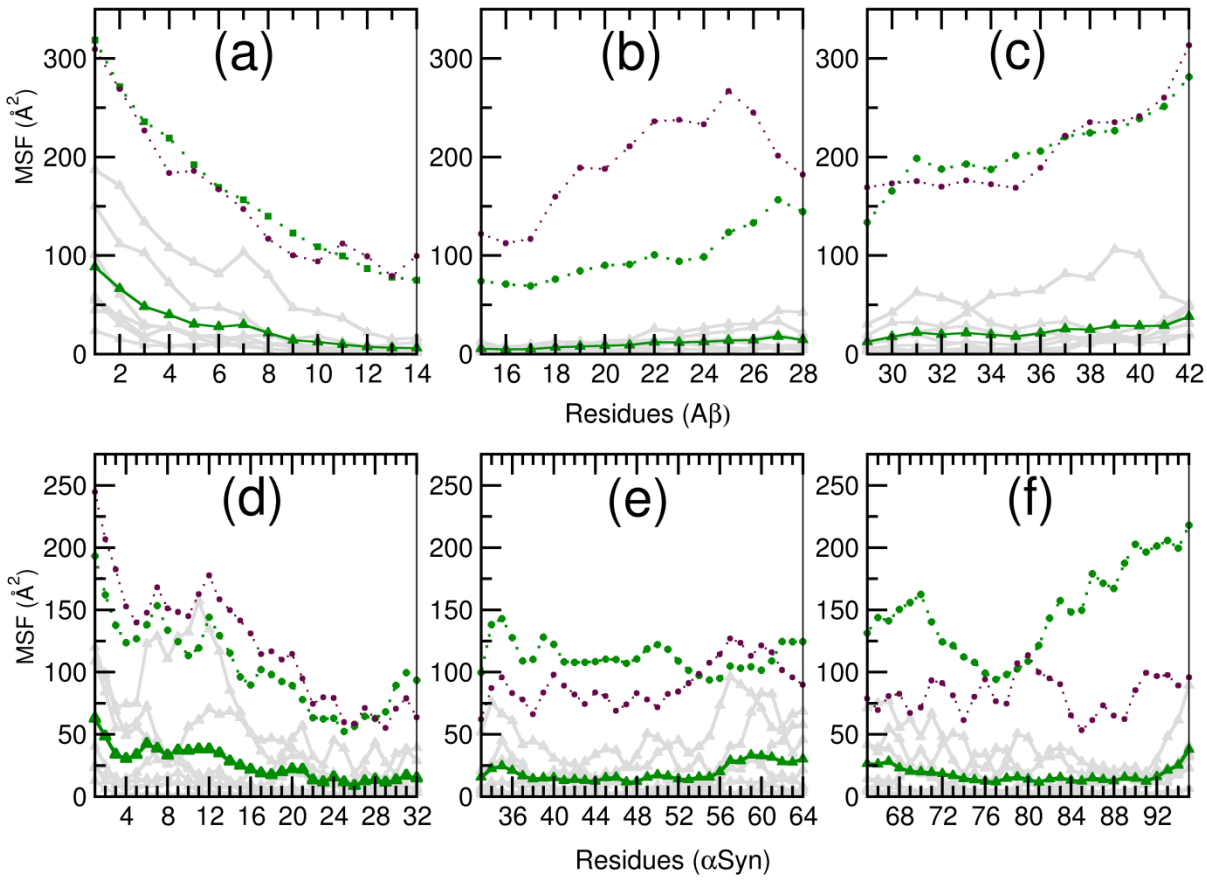

Figure S2. The backbone mean square fluctuation (MSF) for the a) N-terminal residues, b) middle regions, and c) C-terminal residues of $A\beta_{1\text{-}42,}$ and the d) N-terminal residues, e) middle regions, and f) C-terminal residues of $\alpha Syn_{1\text{-}95}$. The data for the last 50 ns of the dimerising trajectories are shown in *gray*, with the averages in *green* (solid line). Corresponding average data for the same systems for the initial 50 ns is provided in green (broken line). Average data for the non-dimerising systems is shown in *maroon* (broken line) for comparison.

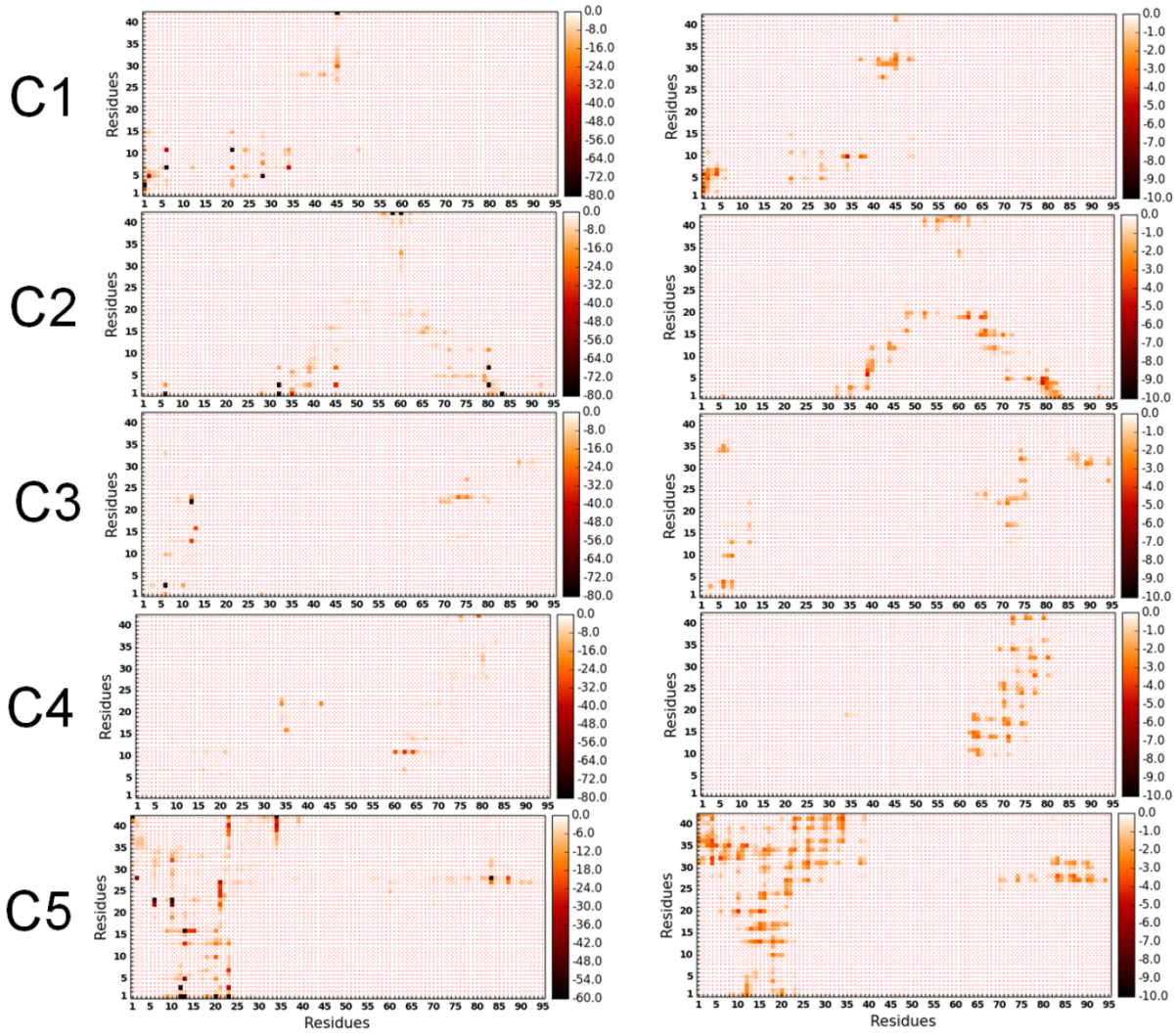

Figure S3. Residue wise maximum electrostatic (left column) and van der Waal (right column) interaction energies (in kcal mol^{-1}) of $\alpha Syn_{1\text{-}95}$ with $A\beta_{1\text{-}42}$ for clusters C1, C2, C3, C4 and C5.