

Electronic Supplementary Information: Pyroglutamate-modified Amyloid β (3-42) Monomer has more β -sheet content than the Amyloid β (1-42) Monomer

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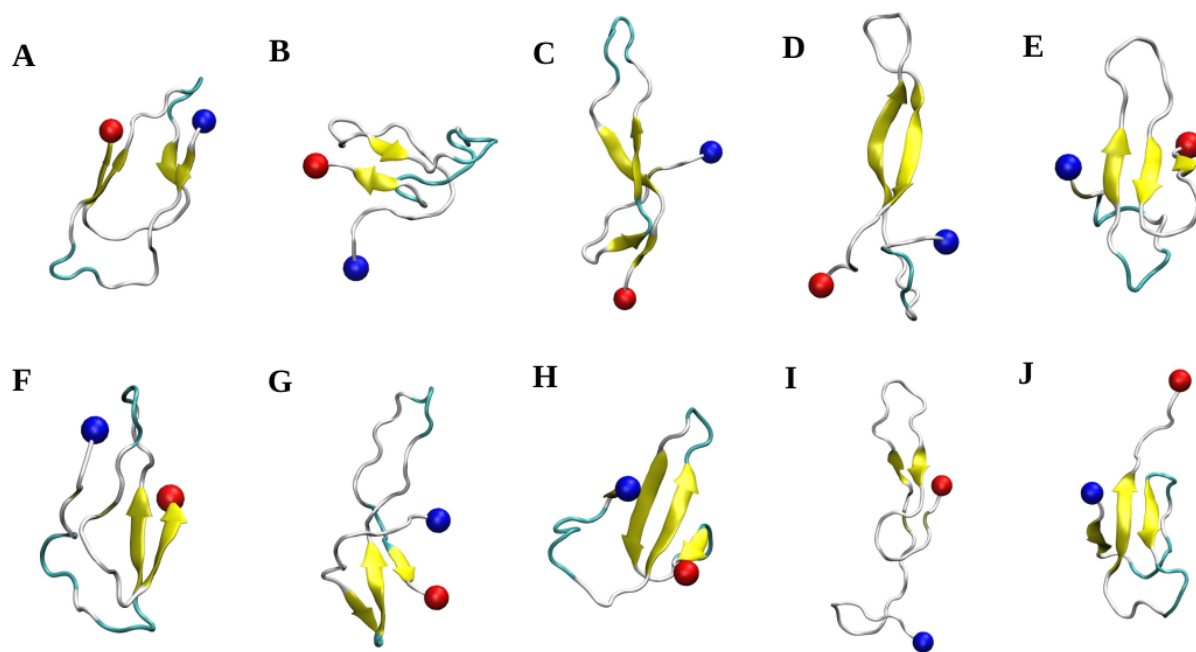


Figure S1 Secondary Structures of Top-10 Clusters of A β (1-42) peptide with N-terminus and C-terminus colored as Blue and Red respectively..

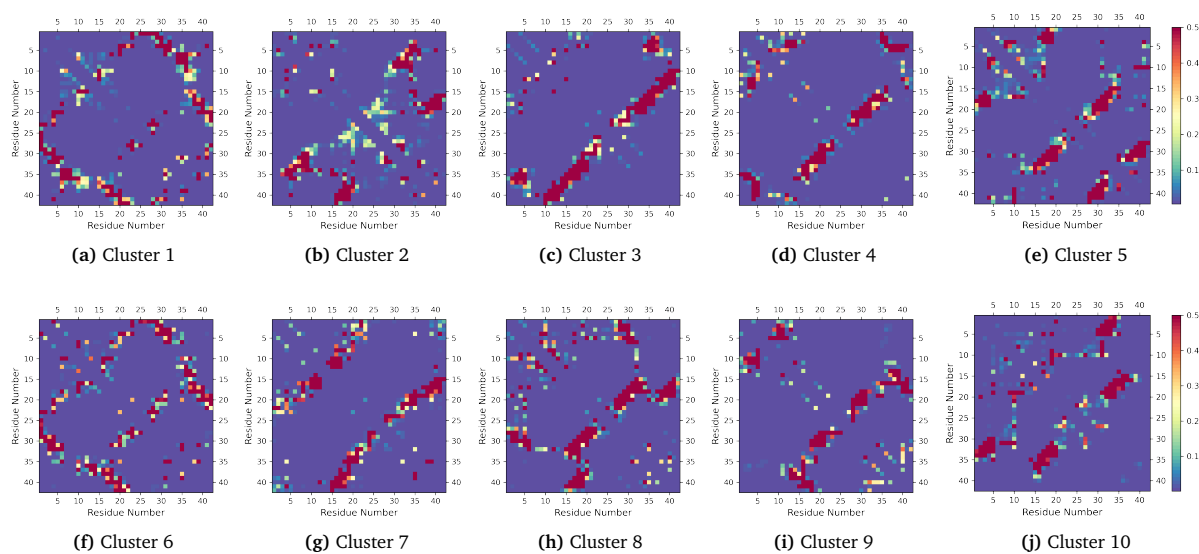


Figure S2 Contact Maps for Top-10 Clusters of A β 1-42 peptide.

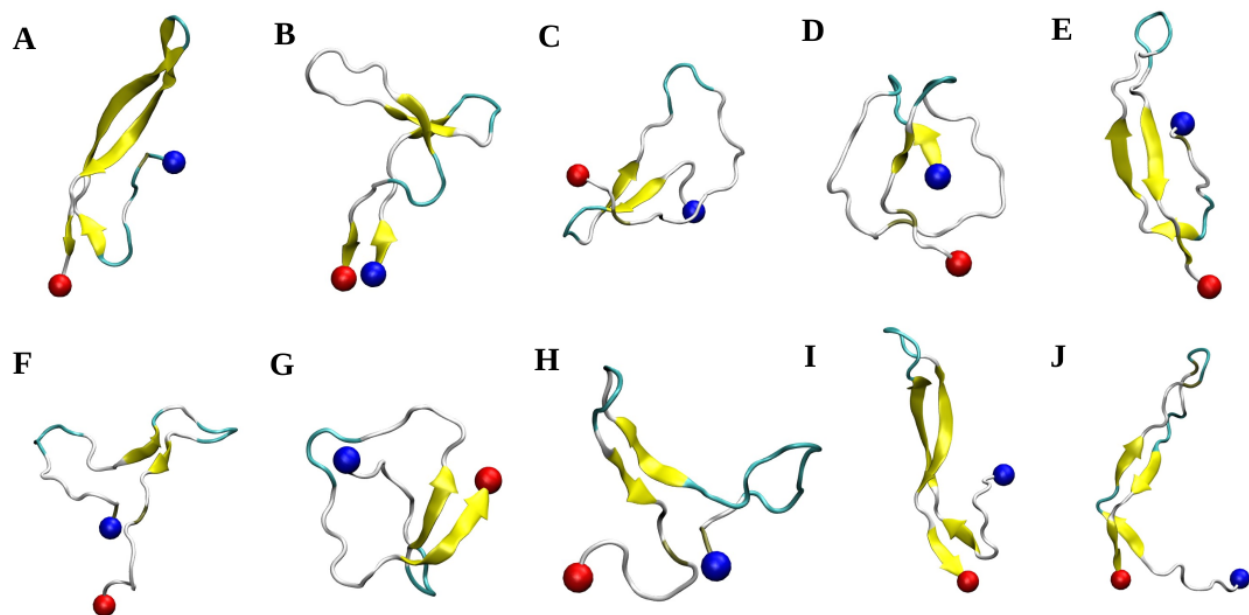


Figure S3 Secondary Structures of Top-10 Clusters of pE-A β (3-42) peptide with N-terminus and C-terminus colored as Blue and Red respectively.

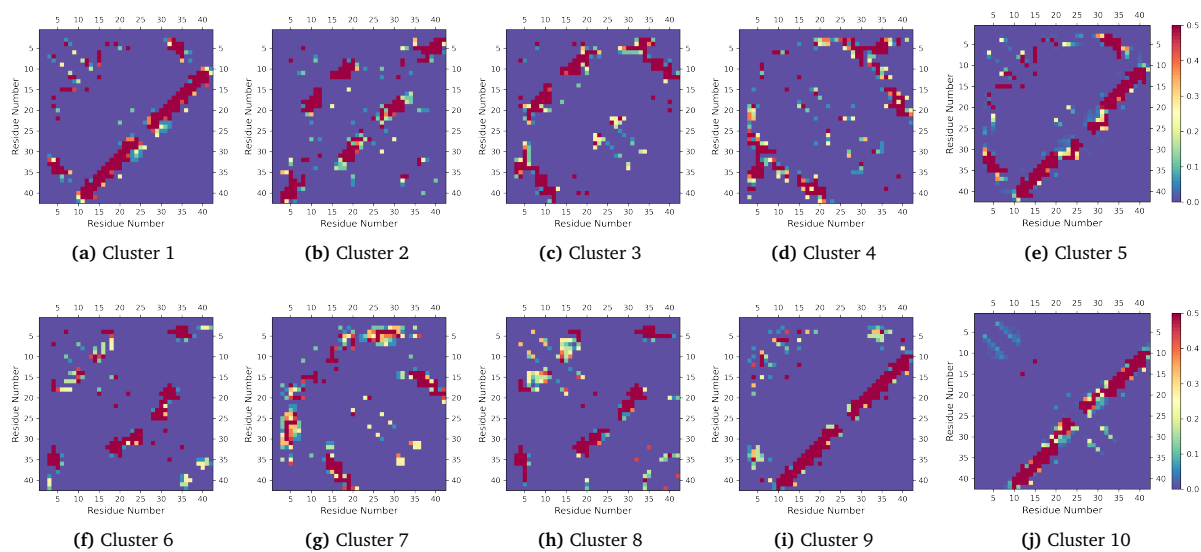


Figure S4 Contact Maps for Top-10 Clusters of pE-A β (3-42) peptide.

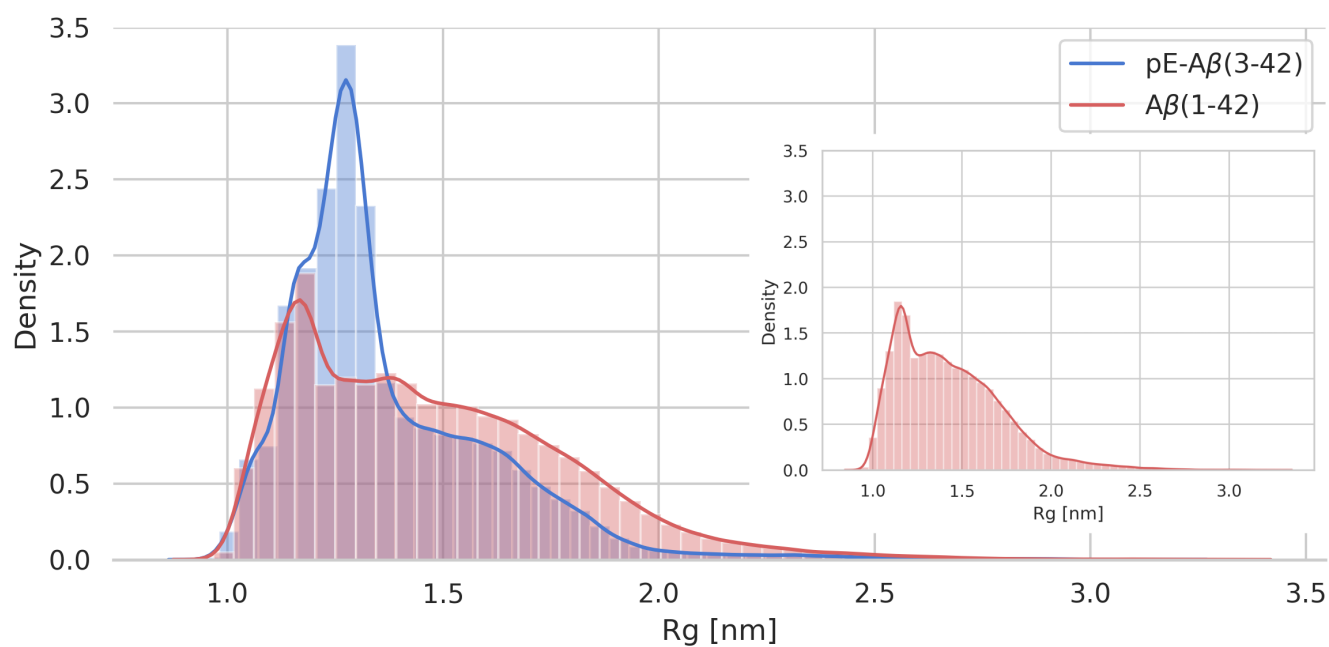


Figure S5 Radius of Gyration (Rg) distribution for pE-A β (3-42) and A β (1-42). The inset shows the distribution for A β (1-42) considering only amino acids 3-42.

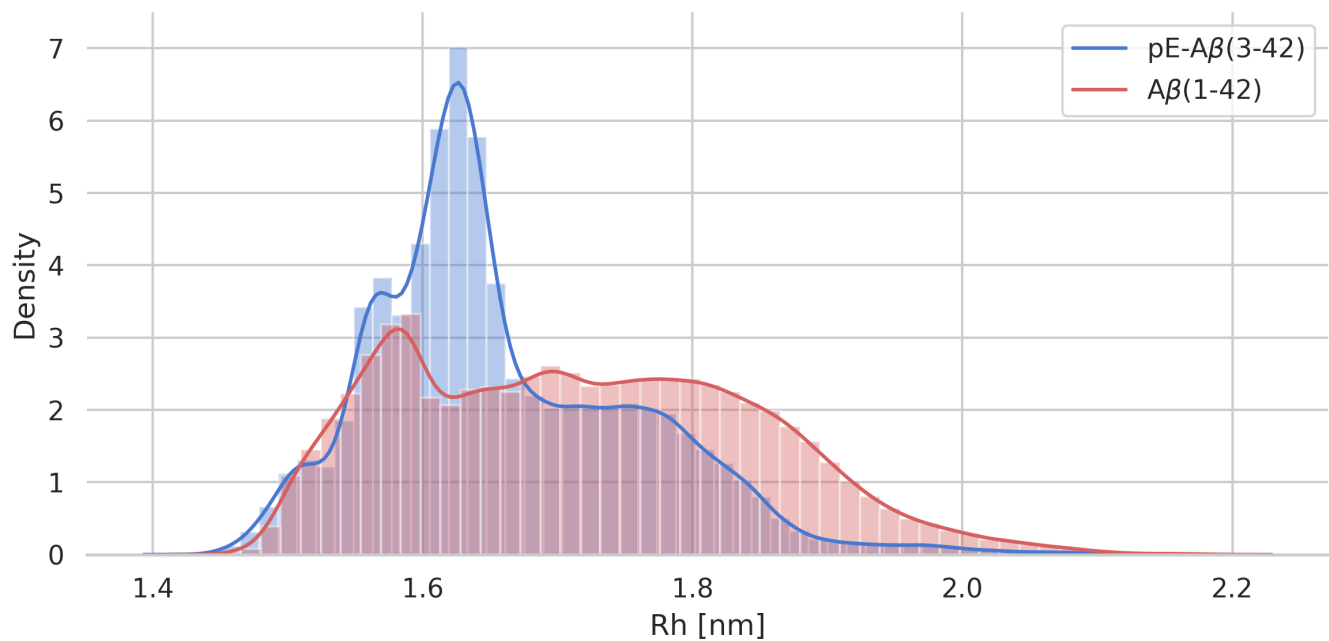


Figure S6 Hydrodynamic Radius (Rh) distribution for A β (1-42) and pE-A β (3-42).

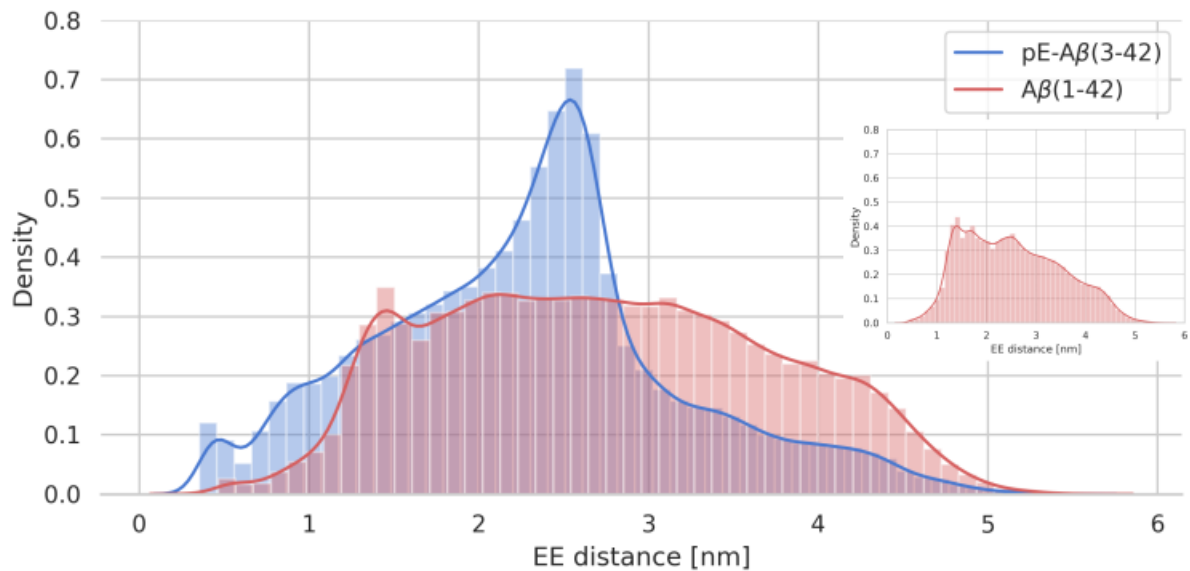


Figure S7 End-to-End (EE) distribution for pE-A β (3-42) and A β (1-42). The inset shows the distribution for A β (1-42) considering only amino acids 3-42.

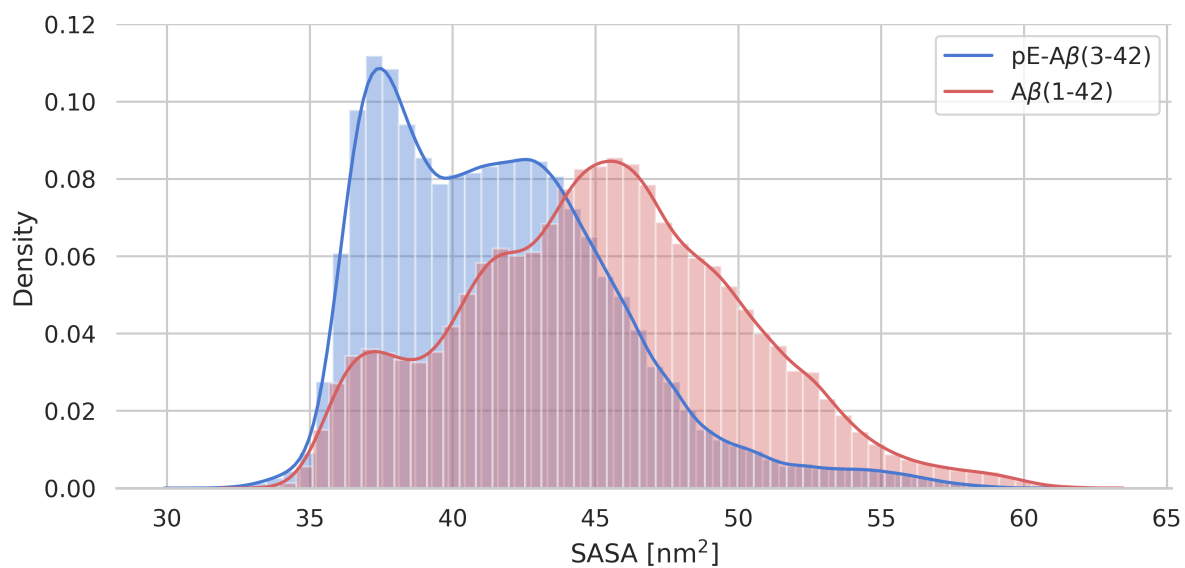


Figure S8 Solvent Accessible Surface Area (SASA) distribution for pE-A β (3-42) and A β (1-42).

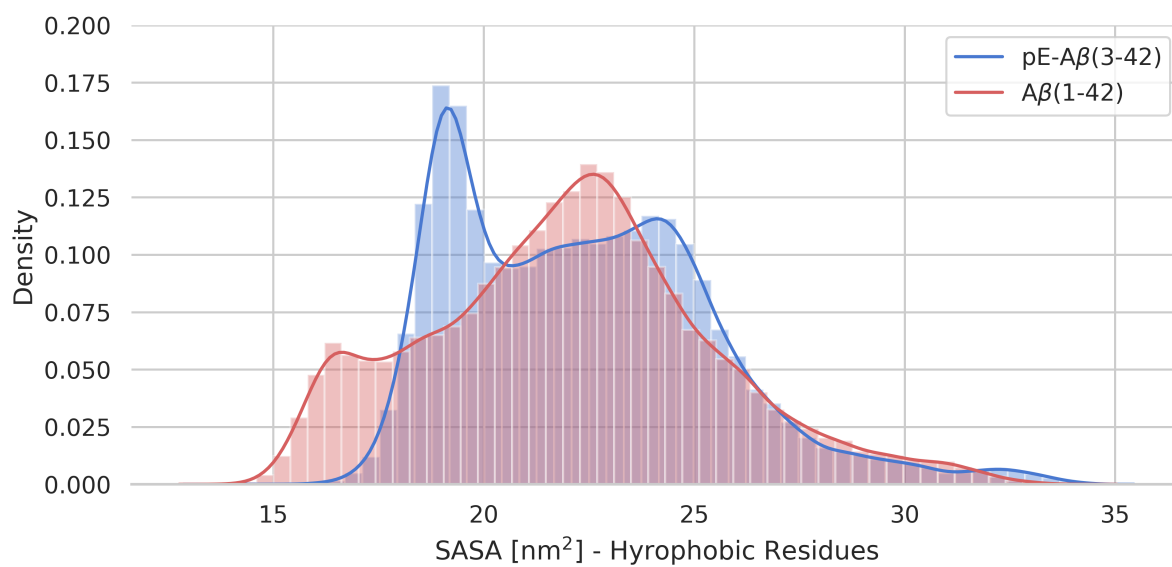


Figure S9 Solvent Accesible Surface Area (SASA) distribution for hydrophobic residues of pE-Aβ(3-42) and Aβ(1-42).

Table S1 Cluster Occurance Probability for A β (1-42) and pE-A β (3-42)

Cluster#	A β (1-42)	pE-A β (3-42)
Cluster 1	6.08 %	18.38 %
Cluster 2	3.38 %	3.86 %
Cluster 3	0.95 %	2.14 %
Cluster 4	0.92 %	1.79 %
Cluster 5	0.91 %	1.36 %
Cluster 6	0.87 %	1.22 %
Cluster 7	0.66 %	1.00 %
Cluster 8	0.56 %	0.96 %
Cluster 9	0.55 %	0.75 %
Cluster 10	0.52 %	0.62 %