SUPPLEMENTAL MATERIAL

Structure and dynamics of parallel β-sheets, hydrophobic core, and loops in Alzheimer's Aβ fibrils

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Fig. S1. The conformations of the infinite fibril segments for the S1, S2 and S3 systems after 10 ns of MD at 298 K. Top views of systems (A) S1-C_{2z}, (B) S1-C_{2x}, (C) S2-C_{2z}, and (D) S3-C_{2z}. Lateral view of systems (E) S1-C_{2z}, (F) S1-C_{2x}, (G) S2-C_{2z}, and (H) S3-C_{2z}.

Fig. S2. Secondary structure of the S2-C_{2z} system along MD trajectories at (A) 298 K and (B) 398 K. Boxed regions indicate formation of helical structure (black).

Fig. S3. Secondary structure of the S3-C_{2z} system along MD trajectories at (A) 298 K and (B) 398 K.

Fig. S4. Structures of Aβ_{1-40} dodecameric fibril segments during the NPT MD simulations at 298, 348 and 398 K. System S1-C_{2z} with -0.5 initial staggering.

Fig. S5. Structures of Aβ_{1-40} dodecameric fibril segments during the NPT MD simulations at 298, 348 and 398 K. System S1-C_{2x} with +0.5 initial staggering.

Fig. S6. Structures of Aβ_{1-40} dodecameric fibril segments during the NPT MD simulations at 298, 348 and 398 K. System S2-C_{2z} with -1.5 initial staggering.

Fig. S7. Structures of Aβ_{1-40} dodecameric fibril segments during the NPT MD simulations at 298, 348 and 398 K. System S2-C_{2z}-AGAA with -1.5 initial staggering and mutations V24A, S26A and N27A.

Fig. S8. Structures of Aβ_{1-40} dodecameric fibril segments during the NPT MD simulations at 298, 348 and 398 K. System S3-C_{2z} with -1.5 initial staggering.

Figures

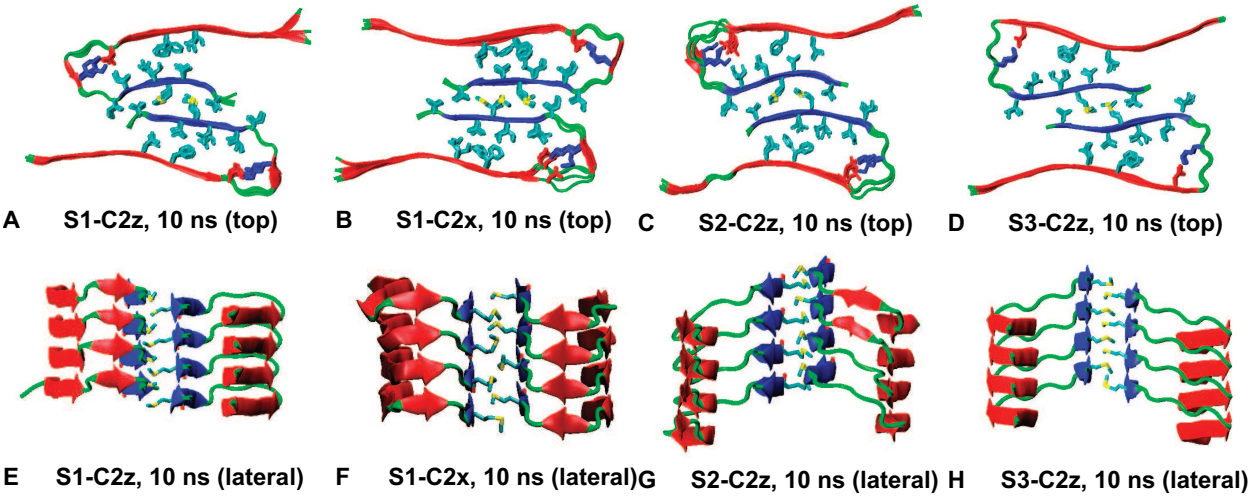

Fig. S 1:

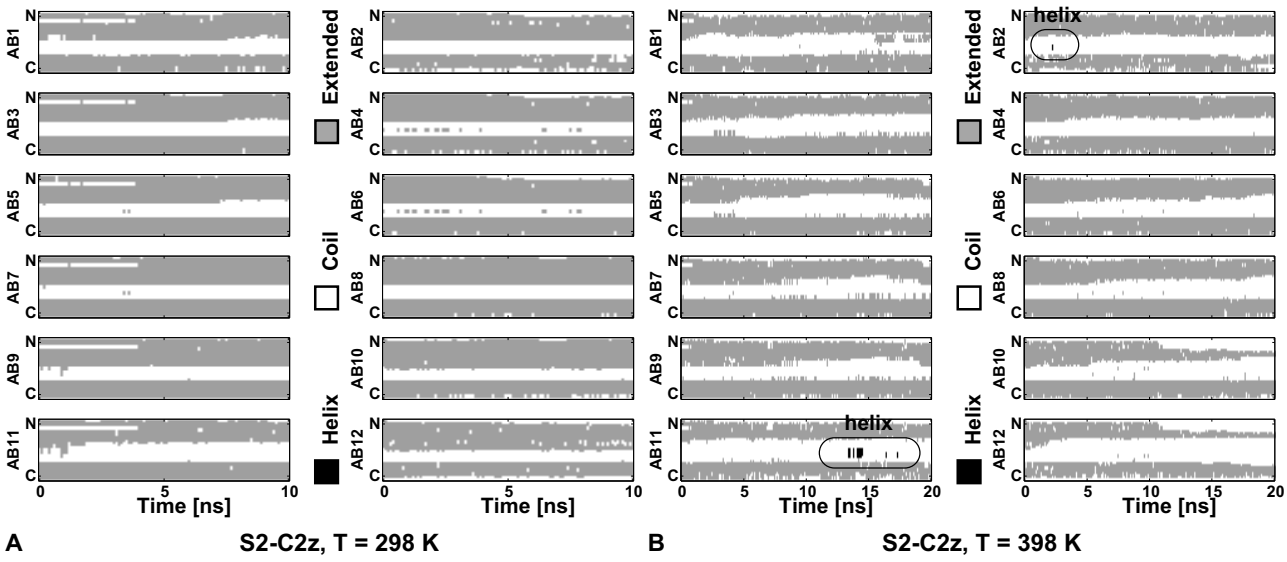

Fig. S 2:

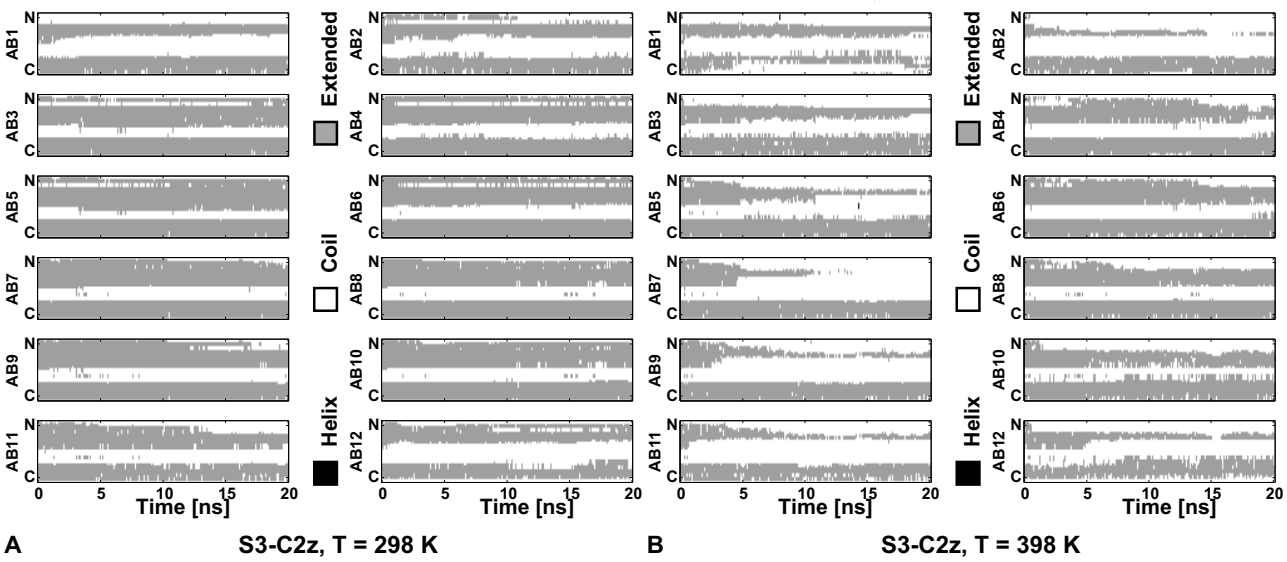
AB1
AB2
AB3
AB4
AB5
AB6
AB7
AB8
AB9
AB10
AB11
AB12
N
C
Extended
Coil
Helix
0
5
10
15
20
Time [ns]
A
S3-C2z, T = 298 K
B
S3-C2z, T = 398 K

Fig. S 3:

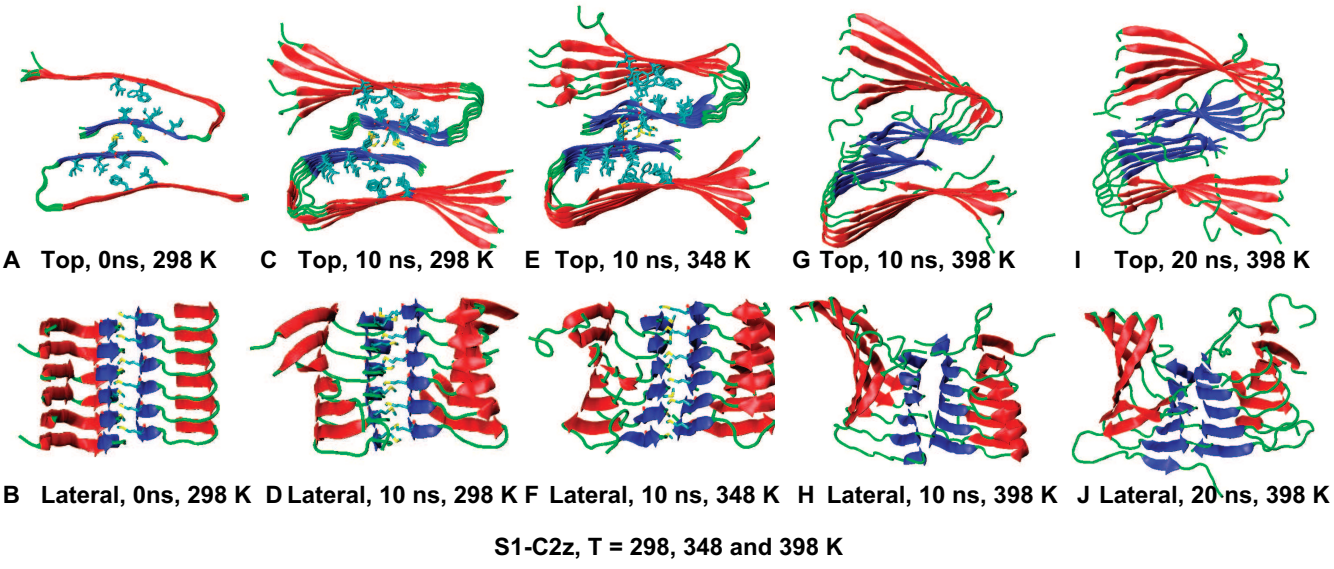
A Top, 0ns, 298 K
C Top, 10 ns, 298 K
E Top, 10 ns, 348 K
G Top, 10 ns, 398 K
I Top, 20 ns, 398 K
B Lateral, 0ns, 298 K
D Lateral, 10 ns, 298 K
F Lateral, 10 ns, 348 K
H Lateral, 10 ns, 398 K
J Lateral, 20 ns, 398 K
S1-C2z, T = 298, 348 and 398 K

Fig. S 4:

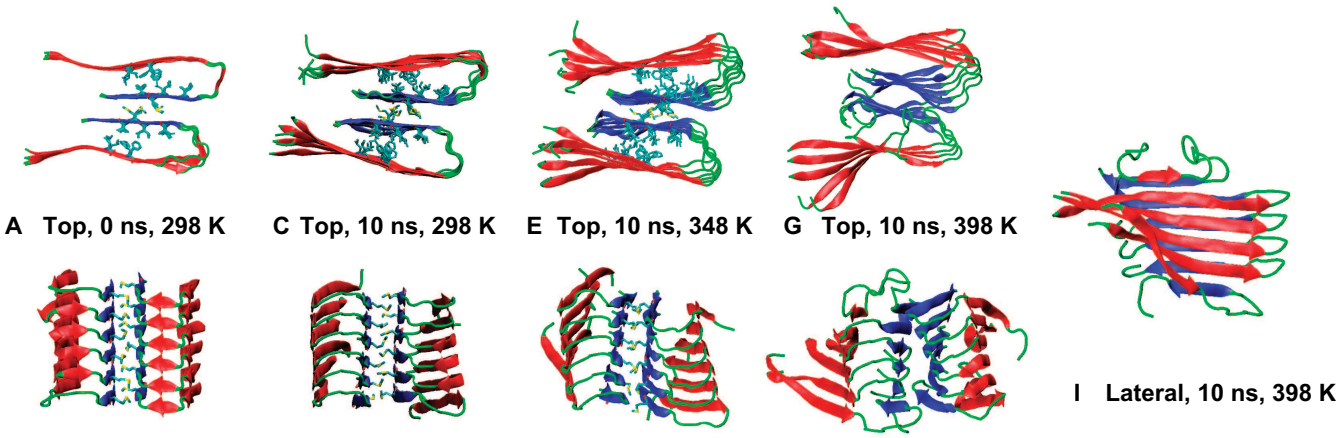
A Top, 0 ns, 298 K
C Top, 10 ns, 298 K
E Top, 10 ns, 348 K
G Top, 10 ns, 398 K
I Lateral, 10 ns, 398 K
B Lateral, 0 ns, 298 K
D Lateral, 10 ns, 298 K
F Lateral, 10 ns, 348 K
H Lateral, 10 ns, 398 K
S1-C2x, T = 298, 348 and 398 K

Fig. S 5:

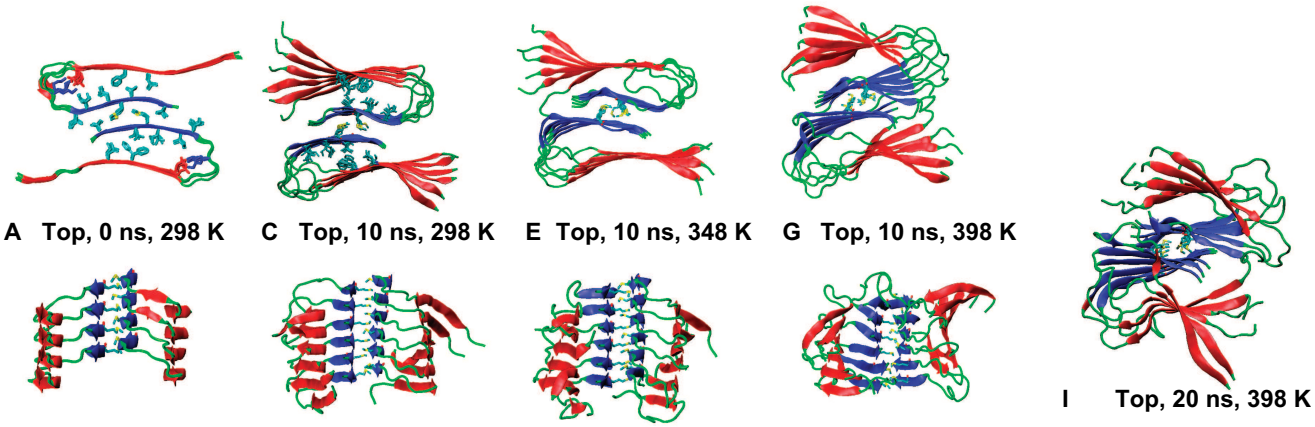
A Top, 0 ns, 298 K
C Top, 10 ns, 298 K
E Top, 10 ns, 348 K
G Top, 10 ns, 398 K
I Top, 20 ns, 398 K
B Lateral, 0 ns, 298 K
D Lateral, 10 ns, 298 K
F Lateral, 10 ns, 348 K
H Lateral, 10 ns, 398 K
S2-C2z, T = 298, 348 and 398 K

Fig. S 6:

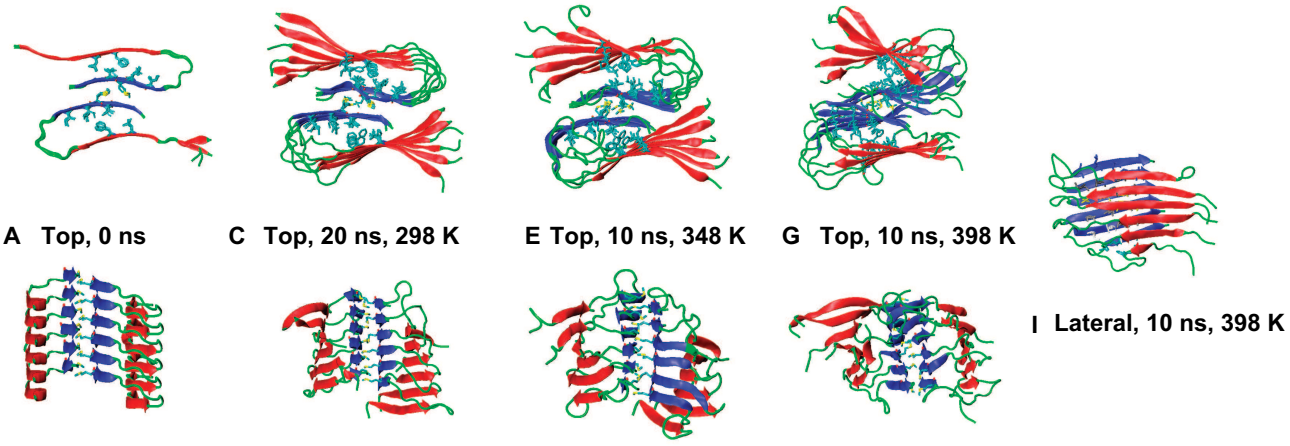
A Top, 0 ns
C Top, 20 ns, 298 K
E Top, 10 ns, 348 K
G Top, 10 ns, 398 K
I Lateral, 10 ns, 398 K
B Lateral, 0 ns
D Lateral, 20 ns, 298 K
F Lateral, 10 ns, 348 K
H Lateral, 10 ns, 398 K
S2-C2z-AGAA, T = 298, 348 and 398 K

Fig. S 7:

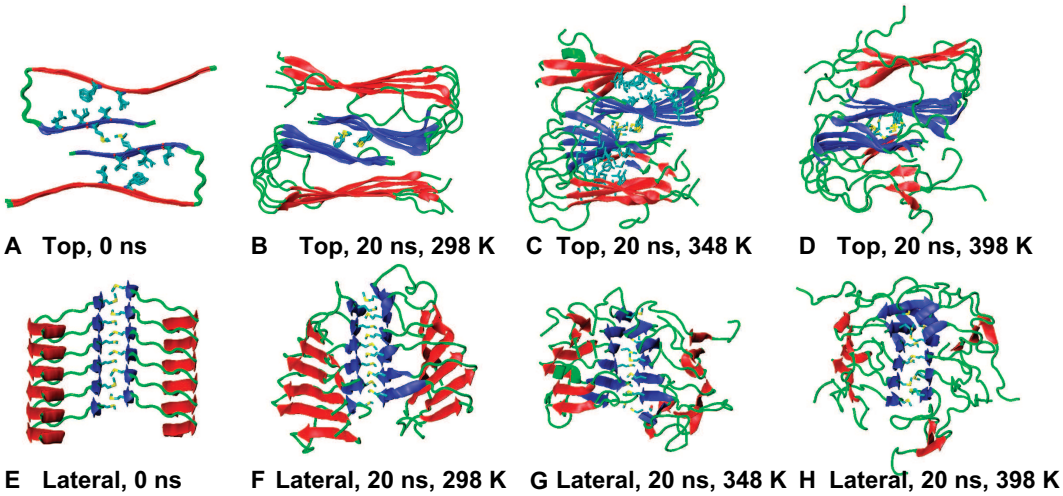
A Top, 0 ns
B Top, 20 ns, 298 K
C Top, 20 ns, 348 K
D Top, 20 ns, 398 K
E Lateral, 0 ns
F Lateral, 20 ns, 298 K
G Lateral, 20 ns, 348 K
H Lateral, 20 ns, 398 K
S3-C2z, T = 298, 348 and 398 K

Fig. S 8: