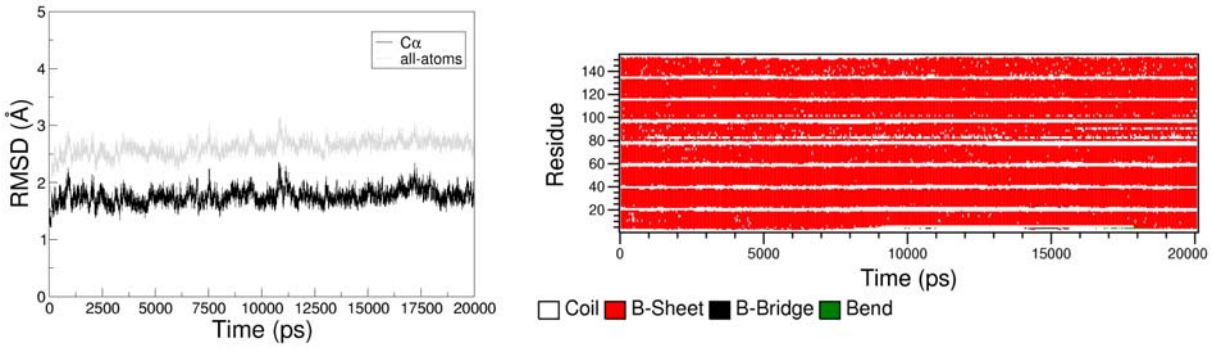
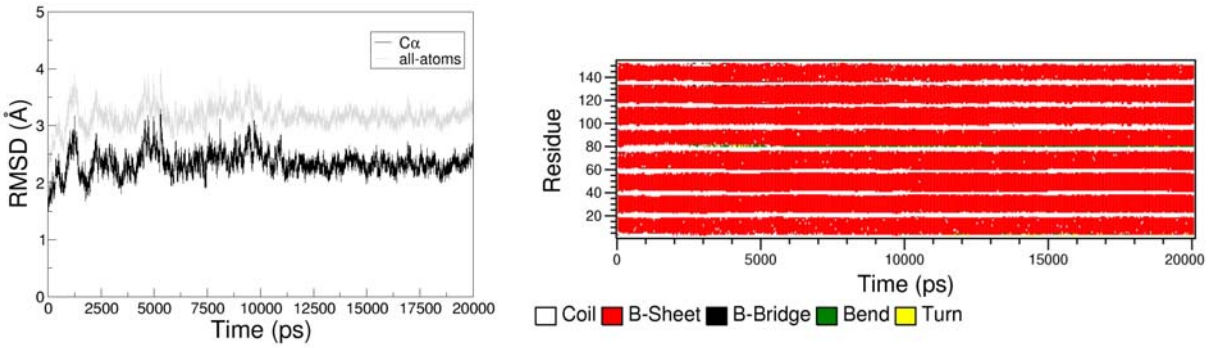
Supplementary Materials



A B

Fig. 1.

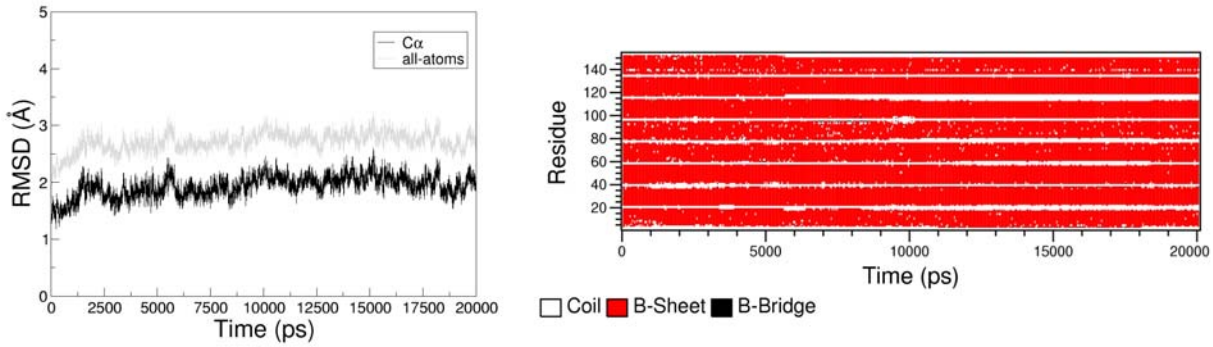
Indicators of htPSH2-ST4-Q15 stability in the MD simulation: (A) root mean square deviations (RMSD), (B) secondary structure.



A B

Fig. 2.

Indicators of hhPSH2-ST4-Q15 stability in the MD simulation: (A) root mean square deviations (RMSD), (B) secondary structure.



A B

Fig. 3.

Indicators of ASH2-ST4-Q15 stability in the MD simulation: (A) root mean square deviations (RMSD), (B) secondary structure.

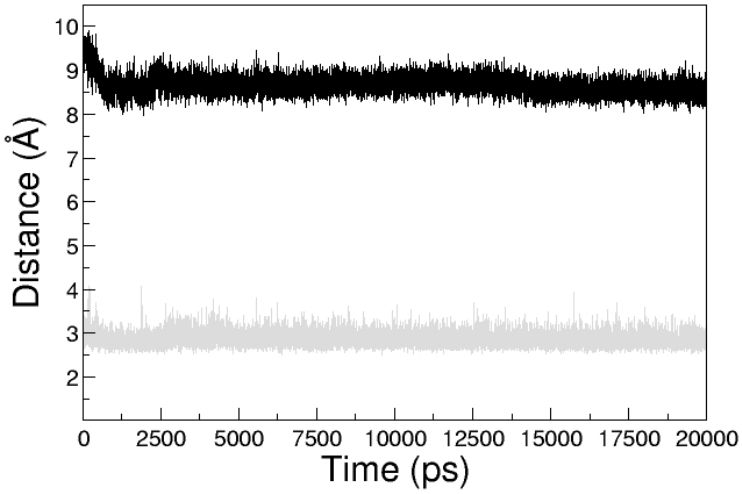


Fig. 4.

Simulation of htPSH2-ST4-Q15 by using the OPLS force field: evolution of C^{α}-C^{α} (black) and main-chain side-chain H-bonding interactions (grey) between representative facing Gln residues in the steric zipper interface.

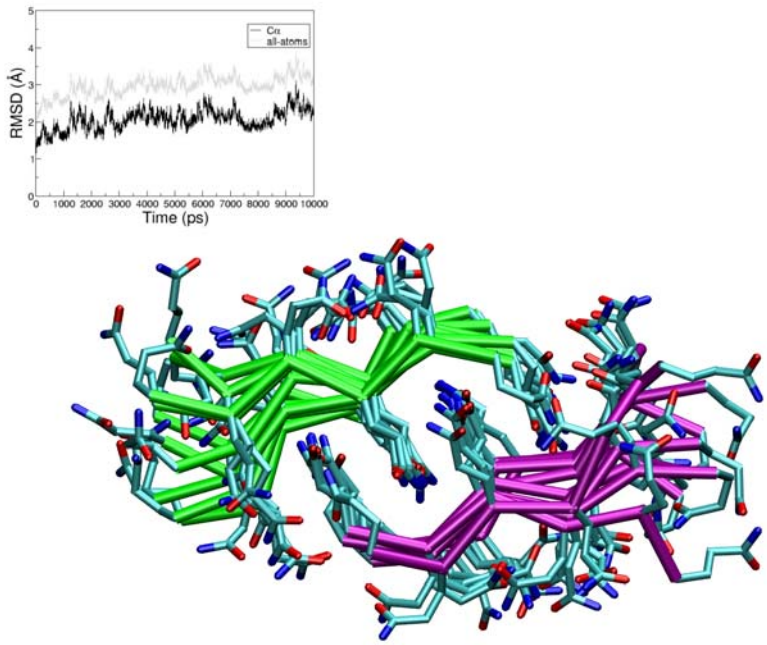


Fig. 5.

Average model of htPSH2-ST10-Q6 derived from the MD trajectory (2000-10000 ps). The RMSD of structures of the trajectory *versus* the starting model is reported in the inset.

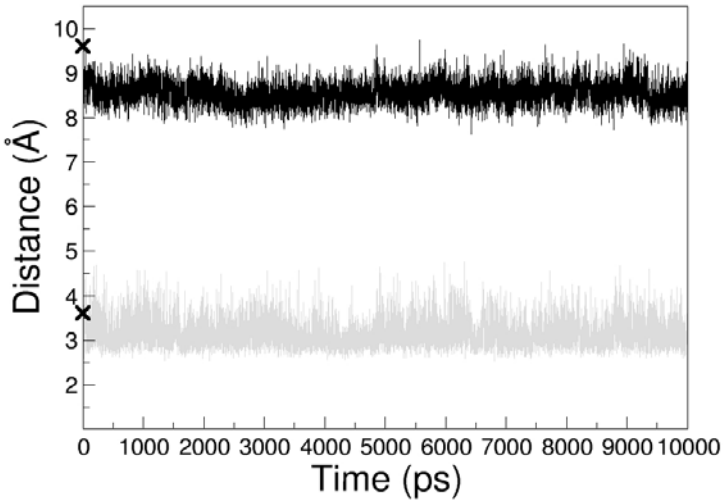


Fig. 6.

Simulation of ASH2-ST10-Q6: evolution of C^{α}-C^{α} (black) and main-chain side-chain H-bonding interactions (grey) between representative facing Gln residues in the steric zipper interface. The black cross on the y axis represent the initial values.

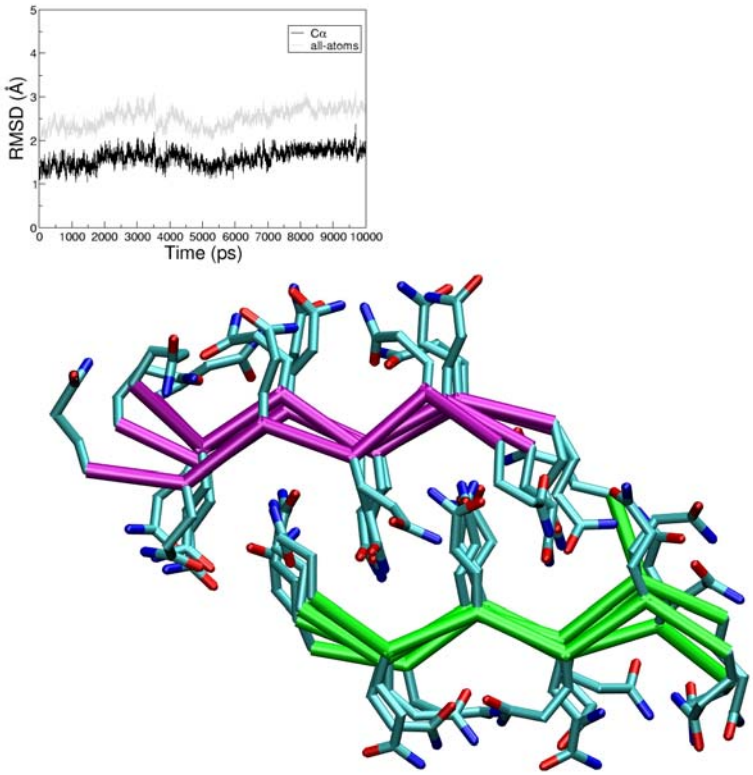


Fig. 7.

Average model of htPSH2-ST4-Q6 derived from the MD trajectory (2000-10000 ps). The RMSD of structures of the trajectory *versus* the starting model is reported in the inset.

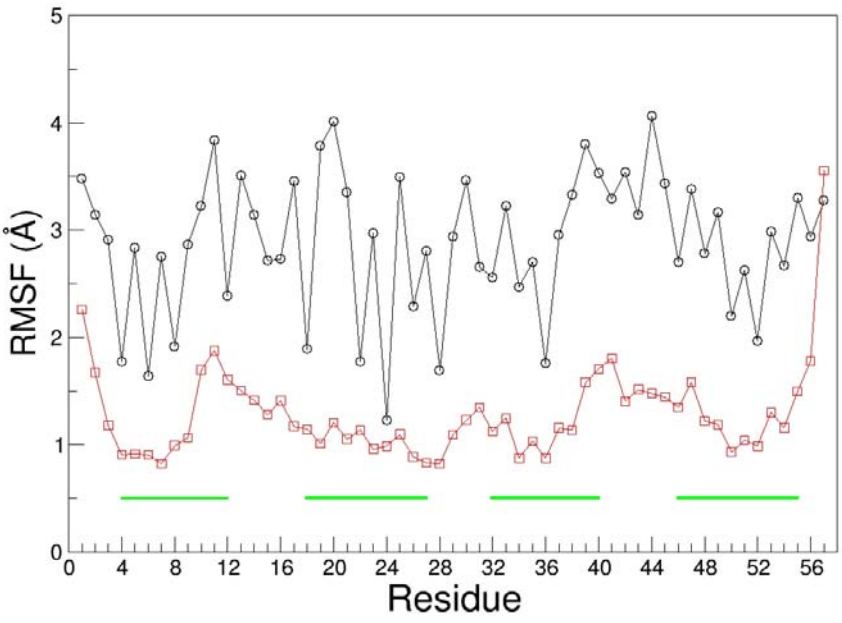


Fig. 8.

Root mean square fluctuation of Gln residues in Q57. Fluctuations calculated on side chain atoms and backbone atoms are shown in black and red, respectively. The green marks correspond to residues located in β-strand regions. The equilibrated region of the trajectory (5000-50000 ps) was considered.

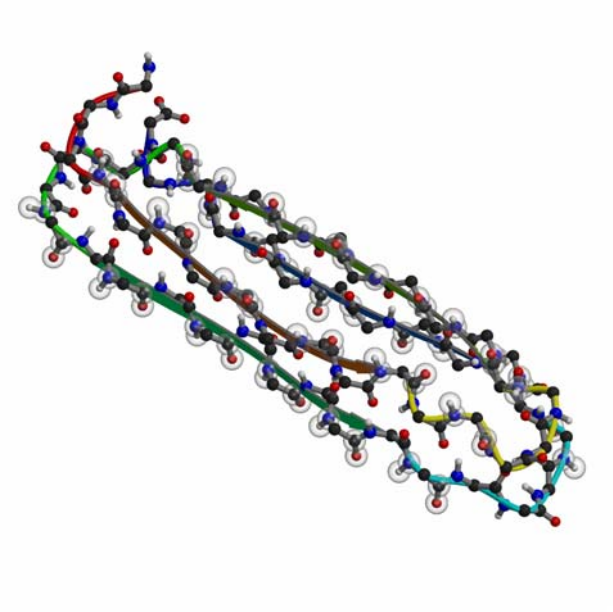


Fig. 9.

Schematic representation of the potentially reactive backbone atoms. For clarity, side chain atoms have been omitted.