Supplementary data

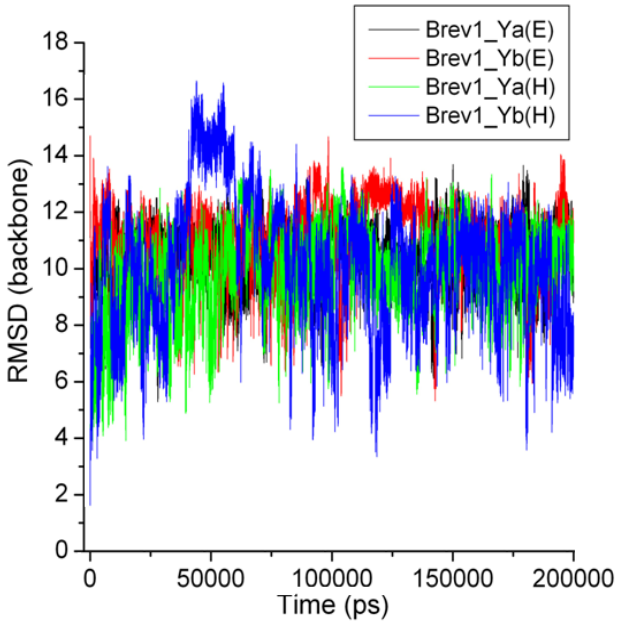



**Figure S(A):** The root mean square deviation (RMSD, Å) of sampled conformations in different simulations relative to their α-helical starting structures.

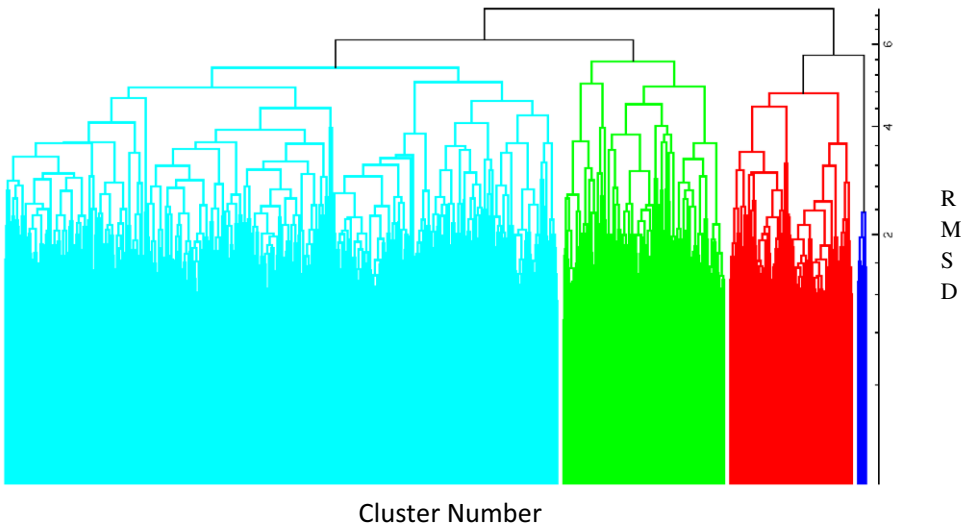



**Figure S(B):** Dendrogram showing different clusters in simulation Brev1_Ya$^{(H)}$.

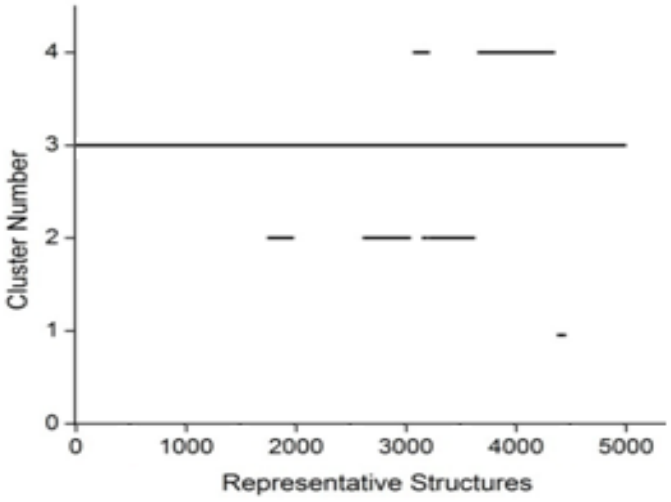



**Figure S(C):** The evolution of 4 clusters across the representative structures for simulation Brev1_Ya$^{(H)}$.

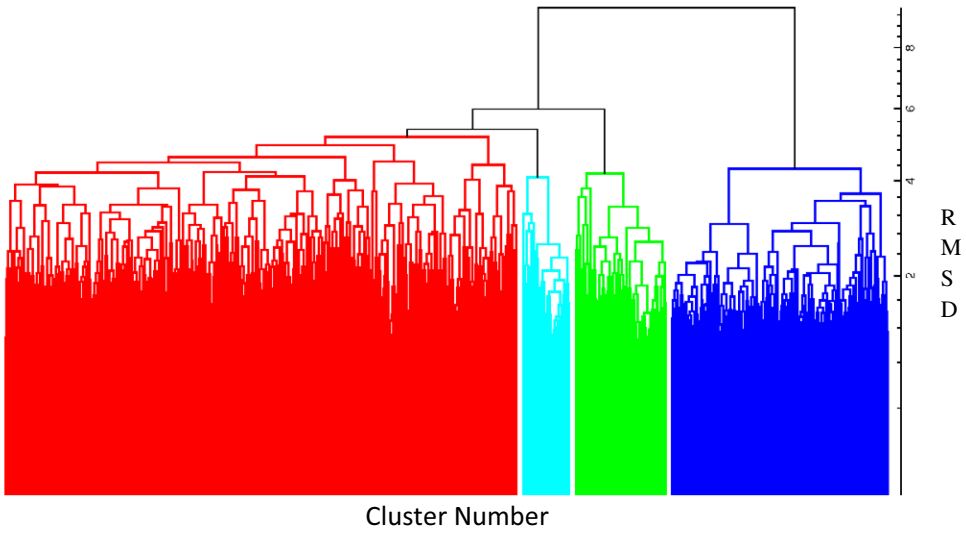



**Figure S(D):** Dendrogram showing different clusters in simulation Brev1_Yb$^{(H)}$.

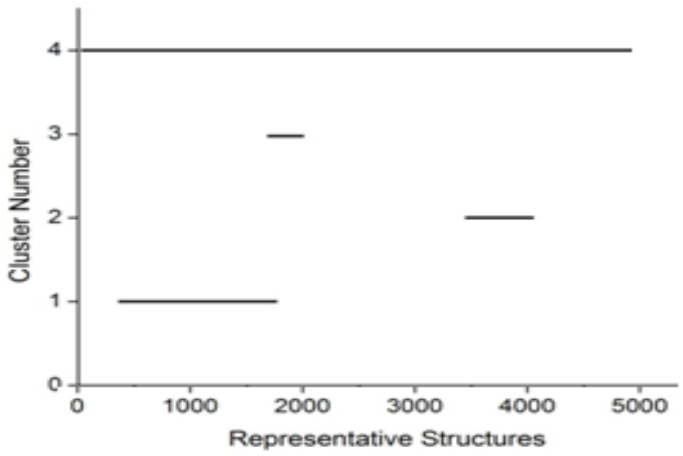



**Figure S(E):** The evolution of 4 clusters across the representative structures in simulation Brev1_Yb$^{(H)}$.

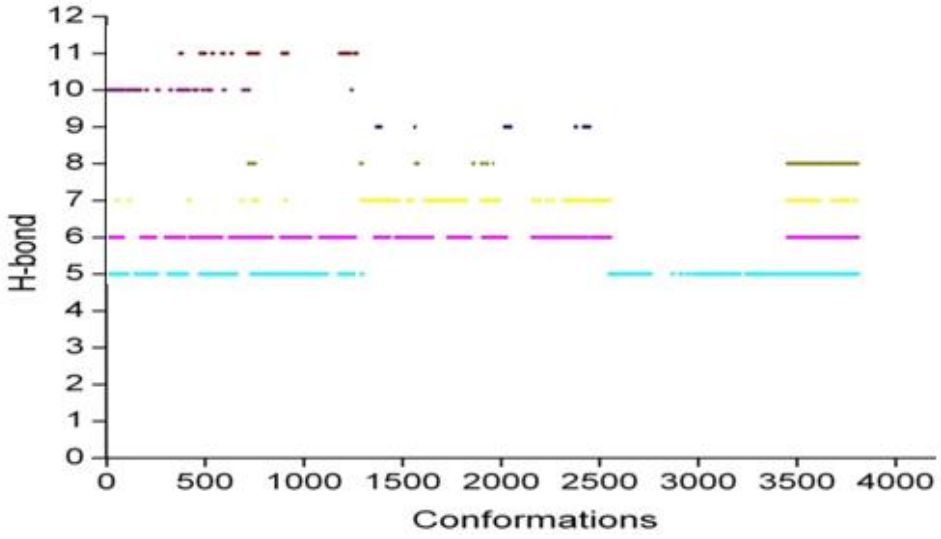



**Figure S(F):** The evolution of intramolecular hydrogen bonds for á-helicity between important residues in the simulation Brev1_Ya$^{(E)}$.

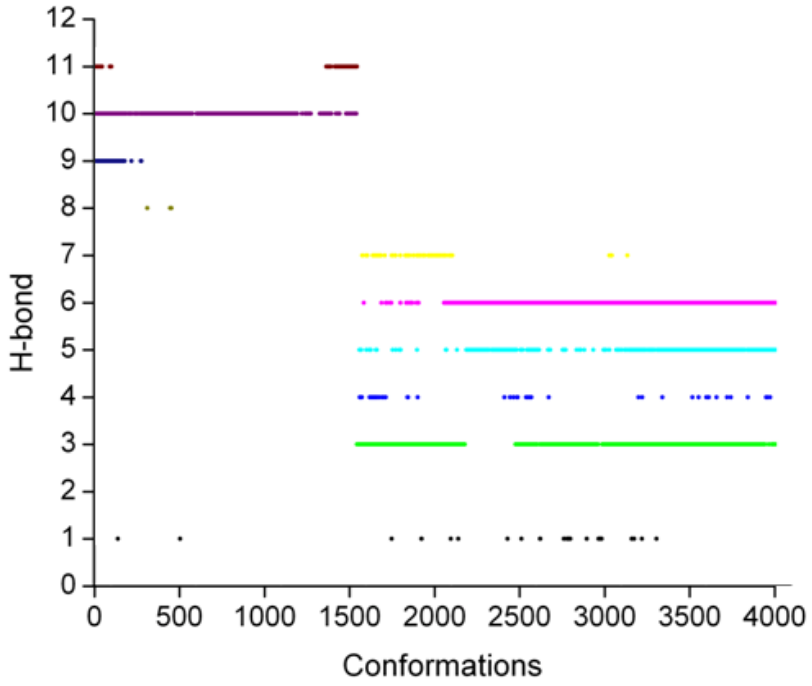



**Figure S(G):** The evolution of intramolecular hydrogen bonds for α-helicity between important residues in the simulation Brev1_Yb$^{(E)}$.

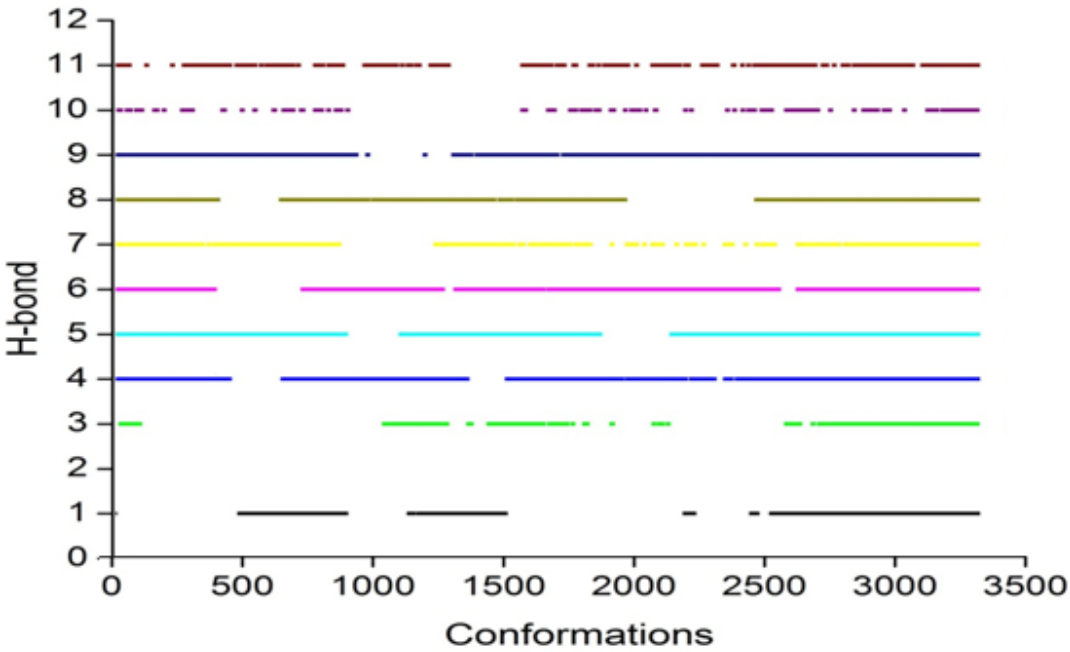



**Figure S(H):** The evolution of intramolecular hydrogen bonds for á-helicity between important residues in the simulation Brev1_Ya$^{(H)}$.

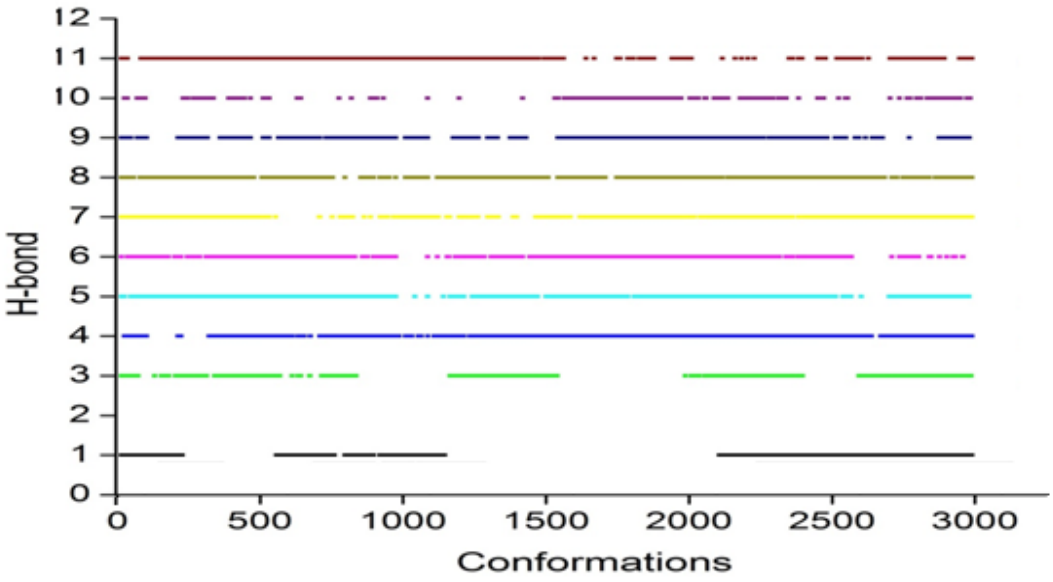
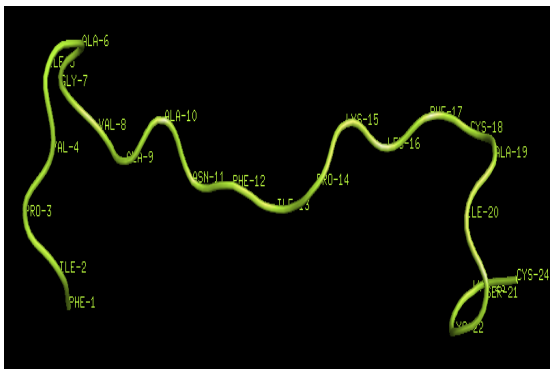



**Figure S(I):** The evolution of intramolecular hydrogen bonds for α-helicity between important residues in the simulation Brev1_Yb$^{(H)}$.

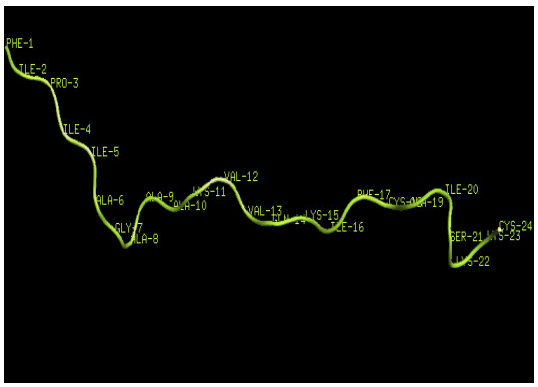
**Table S1:** The α-helical propensities observed due to backbone–backbone hydrogen bond interactions and their percentages in the largest cluster of each trajectory performed.

| Hbond Number | Donor-acceptor | C1 (Brev1_Ya$^{(E)}$) | C1 (Brev1_Yb$^{(E)}$) | C3 (Brev1_Ya$^{(H)}$) | C4 (Brev1_Yb$^{(H)}$) |
|---|---|---|---|---|---|
| 1 | (10)O....N(14) | ---- | 7.2 | 18.5 | 19.2 |
| 2 | (11)O....N(15) | ---- | ---- | ---- | ---- |
| 3 | (12)O....N(16) | ---- | 32.2 | 38.8 | 39.2 |
| 4 | (13)O....N(17) | ---- | 6.1 | 33.1 | 36.3 |
| 5 | (14)O....N(18) | 23.1 | 27.2 | 29.4 | 29.8 |
| 6 | (15)O....N(19) | 29.9 | 30.1 | 35.1 | 35.4 |
| 7 | (16)O....N(20) | 11.2 | 5.3 | 24.7 | 27.2 |
| 8 | (17)O....N(21) | 3.2 | 1.5 | 22.9 | 19.5 |
| 9 | (18)O....N(22) | 3.6 | 4.3 | 18.3 | 20.0 |
| 10 | (19)O....N(23) | 10.8 | 19.4 | 17.1 | 18.1 |
| 11 | (20)O....N(24) | 3.9 | 3.5 | 15.2 | 16.3 |

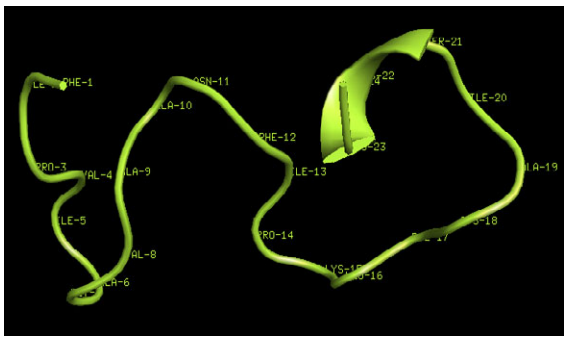
C2 (Brev1_Ya$^{(E)}$)



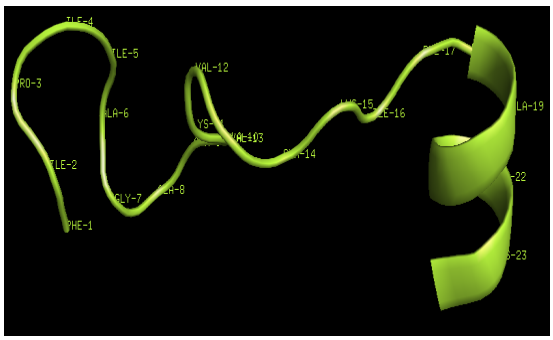

C2 (Brev1_Yb$^{(E)}$)



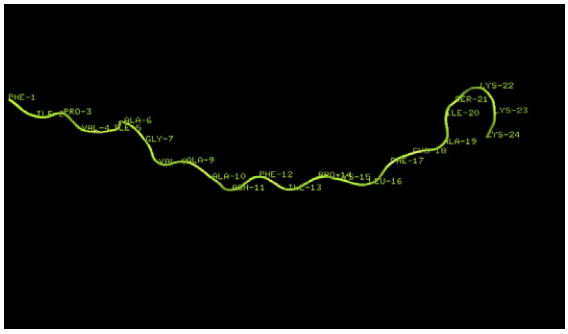

C3 (Brev1_Ya$^{(E)}$)



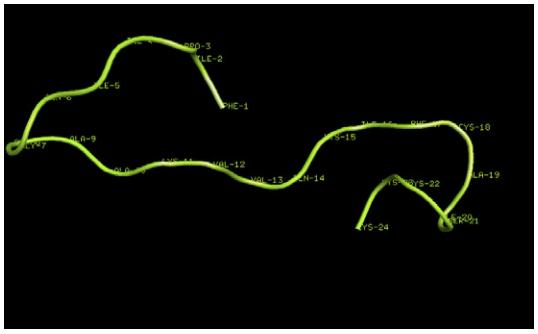

C3 (Brev1_Yb$^{(E)}$)




C4 (Brev1_Ya$^{(E)}$)

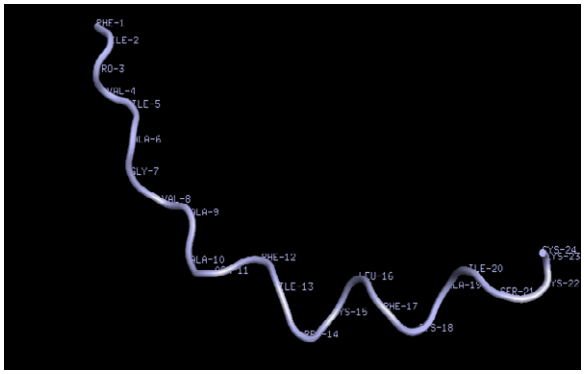


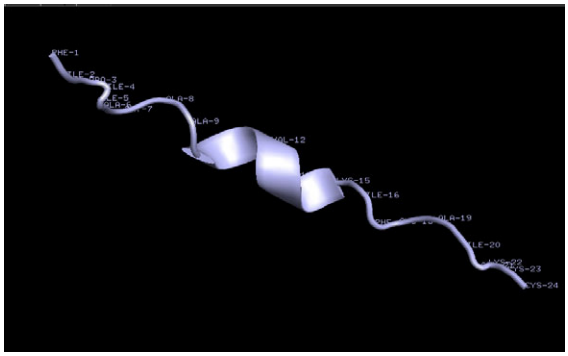

C4 (Brev1_Yb$^{(E)}$)



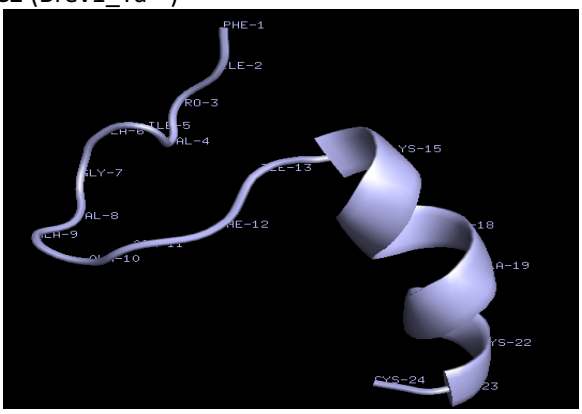

C1 (Brev1_Ya$^{(H)}$)

C1 (Brev1_Yb$^{(H)}$)

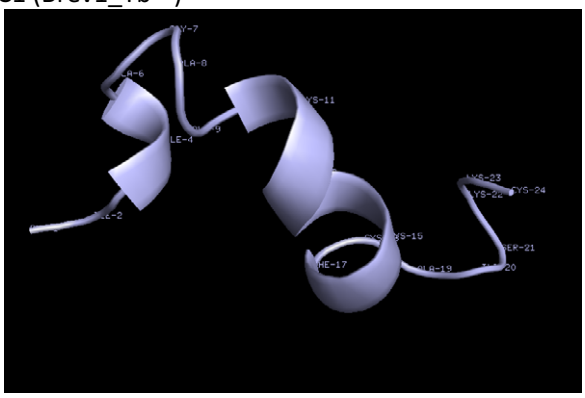




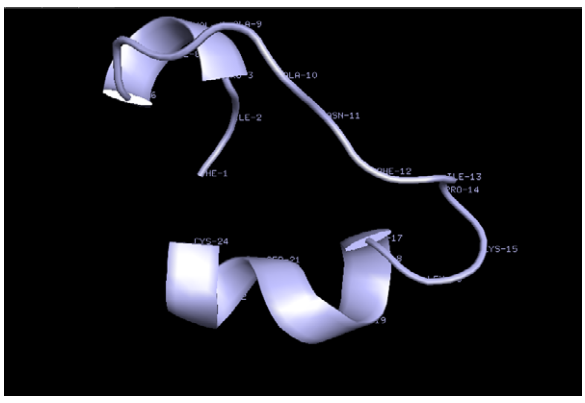
C2 (Brev1_Ya$^{(H)}$)



C1 (Brev1_Yb$^{(H)}$)



C4 (Brev1_Ya$^{(H)}$)



C3 (Brev1_Yb$^{(H)}$)