Supplementary materials

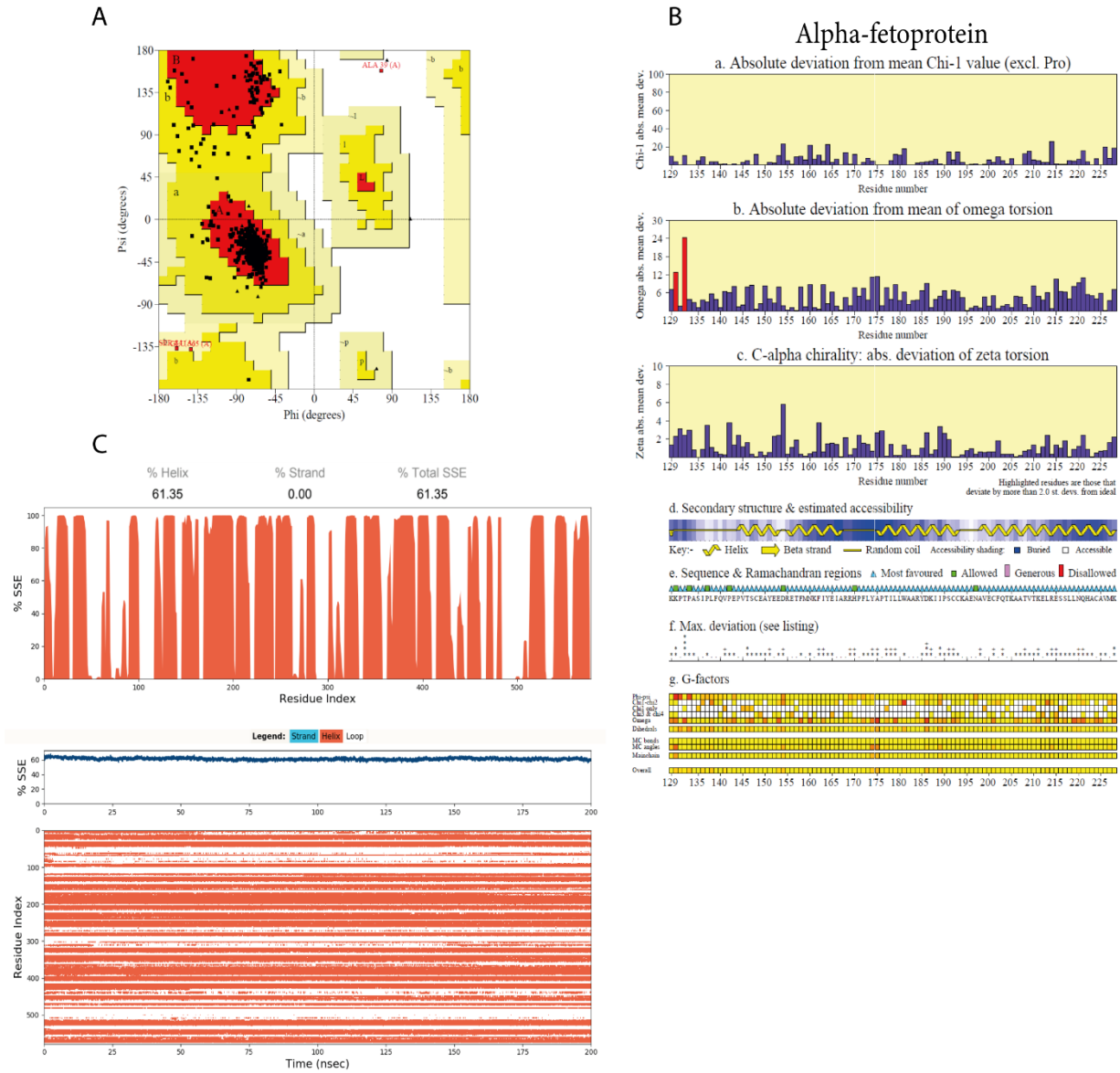

Figure S1. Validation of HAFP 3D model structure obtained based on homology with HSA. (A) Ramachandran map for the main chain conformation shows that 99.5% residues (black dots) are located in favored (red) and allowed (yellow) regions. (B) Graphs and diagrams of stereo-chemical properties of individual residues demonstrate high quality of the model structure. (C) Secondary structure element (SSE) diagrams demonstrate stability of α-helical regions.

Table S1. Experimental binding affinities of estrogens to rat AFP

Ligand	K_a RAFP (M^{-1})	K_d RAFP (M)	ΔG_{RAFP} (kcal/mol)	References
17β-estradiol	From 9.3 x 10^8 To 11.4 x 10^8	From 0.107 x 10^{-8} To 0.088 x 10^{-8}	From -12.232 To -12.347	[31]
17β-estradiol	From 0.6 x10^8 To 1.4 x10^8	From 1.667 x 10^{-8} To 0.714 x 10^{-8}	From -10.606 To -11.106	[42]
17β-estradiol	2.83±0.78 x10^8	0.353 x 10^{-8}	-11.525	[43]
17β-estradiol	5.0 x 10^7	0.200 x 10^{-7}	-9.135	[44]
Estrone	5.51±1.01 x 10^8	0.182 x 10^{-8}	-11.917	[43]
Estrone	9.0 x 10^7	0.111 x 10^{-7}	-10.847	[44]
DES	1.5 x 10^6	0.667 x 10^{-6}	-8.452	[45]

Table S2. Experimental binding affinities of estrogens to mouse AFP

Ligand	K_a MAFP (M^{-1})	K_d MAFP (M)	ΔG_{MAFP} (kcal/mol)	References
17β-estradiol	0.8 x10^8	1.25 x 10^{-8}	-10.777	[46]
DES	0.2 x 10^7	5.00 x 10^{-7}	-8.592	[46]