

Supporting Materials

Probing the U-shaped Conformation of Caveolin-1 in a Bilayer

Huan Rui,^{¶‡} Kyle T. Root,^{‡‡} Jinwoo Lee,[†] Kerney Jebrell Glover,[†] and Wonpil Im^{¶*}

[¶]Department of Molecular Biosciences and Center for Bioinformatics, The University of Kansas, Lawrence, KS and

[†]Department of Chemistry, Lehigh University, Bethlehem, PA

Keywords: Caveolae; Membrane protein conformation and orientation; Protein-lipid interactions

*Corresponding authors:

Wonpil Im: wonpil@ku.edu

Kerney Jebrell Glover: kjg206@lehigh.edu

TABLE S1. Average values of the conformational parameters (θ , ϕ , ρ_1 , ρ_2 , Z_{COM} , α , and β) of Cav1₈₂₋₁₃₆.

	θ	ϕ	ρ_1	ρ_2	Z_{G108} [Å]	Z_{I109} [Å]	Z_{P110} [Å]	α	β
45_1	44°±4°	39°±6°	353°±14°	325°±11°	-6.0±2.1	-7.5±2.3	-9.7±2.1	101°±5°	63°±6°
45_2	63°±11°	14°±7°	334°±17°	116°±10°	-6.5±2.0	-7.1±1.9	-8.3±1.9	109°±7°	51°±9°
45_3	34°±3°	24°±8°	34°±10°	330°±9°	0.7±2.3	-0.4±2.1	2.0±2.2	49°±7°	46°±7°
45_4	12°±5°	28°±7°	327°±14°	328°±12°	-5.4±2.6	-7.7±2.7	-8.8±2.7	76°±6°	66°±5°
45_5	44°±5°	45°±6°	197°±13°	61°±11°	-7.8±1.9	-4.8±1.8	-6.2±1.7	115°±7°	71°±10°
45_6	62°±6°	6°±4°	324°±23°	137°±20°	-6.4±1.9	-7.0±2.0	-8.1±1.8	109°±6°	49°±6°
45_7	30°±3°	7°±5°	41°±9°	341°±9°	-5.0±2.0	-4.7±2.0	-5.1±2.0	64°±6°	60°±6°
45_8	45°±5°	6°±4°	335°±16°	288°±13°	-5.3±2.2	-8.0±2.3	-8.7±2.2	96°±5°	52°±4°
45_9	47°±9°	14°±6°	347°±15°	111°±12°	-5.4±1.9	-6.1±1.8	-8.8±1.8	90°±11°	45°±5°
45_10	29°±3°	13°±4°	217°±28°	112°±8°	-5.5±1.6	-4.7±1.6	-4.5±1.6	73°±6°	68°±6°
Avg. ± S.E.	41°±15°	20°±13°	251°±118°	215°±109°	-5.3±2.1	-5.8±2.2	-6.6±3.3	88°±21°	57°±9°
55_1	66°±12°	18°±6°	262°±19°	308°±13°	-5.2±2.0	-7.3±1.8	-8.0±1.9	121°±9°	55°±8°
55_2	27°±5°	22°±5°	318°±10°	17°±11°	-8.9±1.9	-6.8±1.9	-7.7±2.0	84°±5°	63°±5°
55_3	51°±5°	31°±5°	282°±15°	278°±9°	-5.8±1.6	-6.3±1.7	-5.5±1.8	120°±6°	73°±7°
55_4	59°±6°	25°±8°	354°±14°	334°±14°	-3.4±2.0	-4.0±1.8	-5.0±1.7	106°±5°	47°±5°
55_5	59°±7°	26°±9°	204°±16°	76°±25°	-9.4±2.3	-7.1±2.4	-7.6±2.2	115°±10°	56°±9°
55_6	26°±7°	10°±6°	218°±14°	293°±18°	-6.9±2.3	-7.1±2.1	-6.2±2.0	80°±9°	55°±8°
55_7	45°±7°	5°±4°	231°±18°	294°±12°	-6.5±2.0	-7.6±2.0	-7.8±2.0	98°±8°	54°±6°
55_8	61°±8°	23°±5°	191°±16°	103°±15°	-7.2±1.8	-5.6±2.2	-6.4±2.3	105°±10°	45°±9°
55_9	51°±9°	27°±8°	343°±13°	345°±12°	-2.8±2.2	-3.6±2.1	-4.7±1.9	96°±7°	45°±6°
55_10	23°±4°	17°±5°	344°±17°	274°±12°	-5.0±1.9	-7.1±2.0	-7.3±2.1	84°±7°	74°±7°
Avg. ± S.E.	47°±15°	20°±7°	275°±59°	232°±113°	-6.1±2.0	-6.3±1.3	-6.6±1.2	101°±14°	57°±10°
65_1	67°±6°	19°±7°	331°±13°	121°±10°	-6.4±2.0	-7.0±1.8	-9.5±1.9	108°±8°	42°±8°
65_2	67°±7°	21°±6°	343°±13°	104°±11°	-7.7±1.9	-7.3±2.1	-8.5±2.1	132°±8°	65°±5°
65_3	63°±10°	19°±10°	331°±12°	121°±11°	-6.8±2.1	-7.6±2.1	-9.3±1.9	103°±6°	44°±9°
65_4	84°±8°	13°±6°	202°±13°	76°±12°	-5.2±1.7	-3.5±1.7	-5.6±1.6	126°±5°	43°±8°

65_5	47°±6°	7°±5°	344°±14°	108°±11°	-3.9±1.8	-4.3±1.6	-6.7±1.6	97°±6°	51°±6°
65_6	49°±7°	16°±6°	59°±19°	61°±12°	-2.8±2.4	-3.7±2.2	-6.9±2.1	92°±12°	43°±11°
65_7	66°±6°	12°±7°	221°±12°	133°±10°	-9.0±2.0	-7.1±2.0	-6.6±1.7	123°±10°	59°±8°
65_8	45°±7°	21°±8°	182°±18°	112°±15°	-5.7±2.6	-2.9±2.6	-3.9±2.3	92°±8°	51°±7°
65_9	30°±4°	18°±6°	215°±18°	96°±8°	-8.8±2.0	-6.5±1.9	-6.2±1.9	99°±10°	82°±6°
65_10	61°±7°	6°±4°	350°±15°	108°±10°	-4.5±1.9	-5.2±1.9	-7.7±1.8	101°±5°	40°±7°
Avg. ± S.E.	58°±14°	15°±5°	257°±93°	104°±20°	-6.1±2.0	-5.5±1.7	-7.1±1.6	107°±14°	52°±13°
75_1	68°±7°	28°±10°	39°±19°	77°±11°	-2.9±2.2	-3.3±2.2	-6.4±2.2	107°±8°	39°±6°
75_2	58°±5°	12°±6°	339°±13°	122°±10°	-4.5±2.7	-5.1±2.8	-7.0±2.4	106°±8°	51°±7°
75_3	58°±7°	15°±8°	229°±12°	108°±12°	-8.5±1.7	-6.9±1.8	-7.3±1.8	108°±7°	51°±6°
75_4	63°±7°	24°±8°	288°±14°	322°±15°	-4.6±1.8	-7.0±2.0	-7.6±2.1	120°±7°	57°±6°
75_5	45°±6°	13°±7°	336°±18°	117°±13°	-3.5±1.9	-4.1±2.0	-5.7±1.9	97°±6°	55°±5°
75_6	65°±8°	65°±7°	323°±13°	340°±21°	3.9±3.1	2.4±2.4	4.1±2.6	105°±14°	41°±15°
75_7	53°±7°	9°±5°	229°±29°	286°±13°	-11.0±2.4	-9.7±2.4	-7.8±2.8	108°±11°	55°±8°
75_8	57°±10°	19°±6°	337°±18°	120°±14°	-5.3±2.2	-5.9±2.0	-7.5±2.0	109°±8°	55°±5°
75_9	66°±5°	27°±6°	318°±13°	124°±10°	-5.3±1.6	-6.7±1.4	-8.8±1.5	104°±6°	42°±5°
75_10	79°±8°	29°±6°	353°±13°	118°±14°	-4.1±2.8	-4.5±2.7	-7.2±2.5	116°±9°	38°±6°
Avg. ± S.E.	61°±9°	24°±15°	279°±90°	173°±95°	-4.6±3.7	-5.1±3.0	-6.1±3.5	108°±6°	48°±7°
85_1	73°±6°	20°±10°	347°±16°	16°±12°	-4.5±2.2	-5.3±1.9	-5.8±1.7	100°±7°	27°±4°
85_2	58°±7°	10°±6°	236°±13°	278°±17°	-9.1±2.2	-7.5±2.2	-6.6±2.3	107°±6°	49°±9°
85_3	68°±9°	10°±5°	350°±16°	111°±13°	-4.3±2.2	-4.5±2.0	-6.5±2.2	104°±9°	37°±5°
85_4	75°±9°	49°±4°	280°±12°	6°±13°	1.3±1.6	-2.4±1.6	-4.1±1.5	126°±6°	52°±9°
85_5	143°±9°	27°±11°	260°±15°	44°±37°	1.7±2.4	-0.6±2.4	2.1±2.4	145°±6°	6°±5°
85_6	74°±7°	37°±6°	310°±15°	128°±11°	-4.6±2.0	-5.8±1.8	-8.7±1.7	113°±9°	41°±6°
85_7	61°±5°	8°±5°	350°±18°	121°±10°	-3.8±2.7	-3.8±2.3	-5.5±2.1	104°±5°	45°±5°
85_8	68°±7°	46°±6°	336°±26°	266°±15°	0.2±2.8	2.8±2.2	1.8±1.8	93°±9°	27°±8°
85_9	33°±4°	13°±7°	358°±14°	316°±15°	-8.0±2.1	-9.3±2.1	-10.2±2.0	88°±5°	57°±5°
85_10	48°±5°	18°±6°	79°±17°	43°±17°	-3.5±2.0	-5.6±1.9	-8.6±1.8	80°±10°	35°±8°
Avg. ± S.E.	70°±27°	24°±15°	291°±81°	133°±109°	-3.5±3.4	-4.2±3.3	-5.2±4.0	106°±18°	38°±14°

Total Avg.	$55^{\circ} \pm 20^{\circ}$	$21^{\circ} \pm 12^{\circ}$	$271^{\circ} \pm 92^{\circ}$	$171^{\circ} \pm 109^{\circ}$	-5.1 ± 2.9	-5.4 ± 2.5	-6.3 ± 3.0	$102^{\circ} \pm 17^{\circ}$	$50^{\circ} \pm 13^{\circ}$
1- μ s Simul.	$53^{\circ} \pm 5^{\circ}$	$27^{\circ} \pm 6^{\circ}$	$331^{\circ} \pm 22^{\circ}$	$124^{\circ} \pm 12^{\circ}$	-5.9 ± 1.7	-6.8 ± 1.6	-9.3 ± 1.3	$99^{\circ} \pm 7^{\circ}$	$49^{\circ} \pm 7^{\circ}$

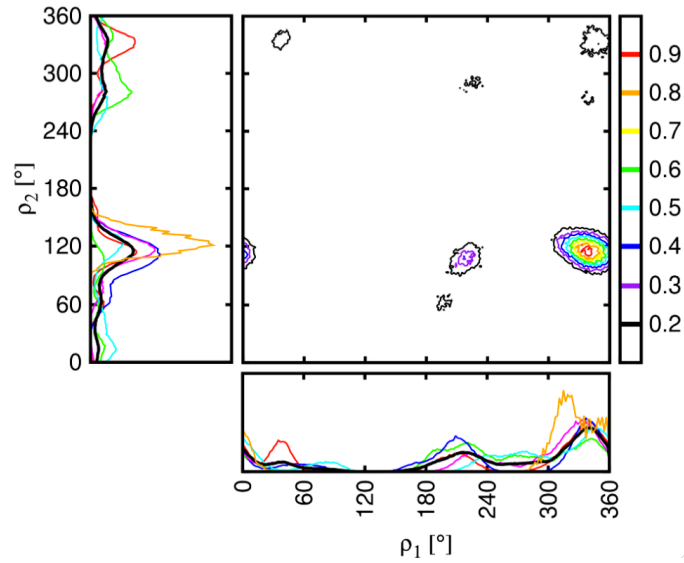


FIGURE S1. The average two-dimensional ρ_1 and ρ_2 distribution from all the multiple simulations shown as a contour map. The contour levels are indicated by different colors, and the color scale goes from black to red denoting population increase. The bottom and left panels show the distributions of ρ_1 and ρ_2 , respectively. The distributions from different systems are distinguished by colors with system cav1_45 in red, cav1_55 in green, cav1_65 in blue, cav1_75 in magenta, cav1_85 in cyan, and the 1- μ s simulation in orange. The averaged one-dimensional ρ_1 and ρ_2 distributions from the multiple simulations are in black.

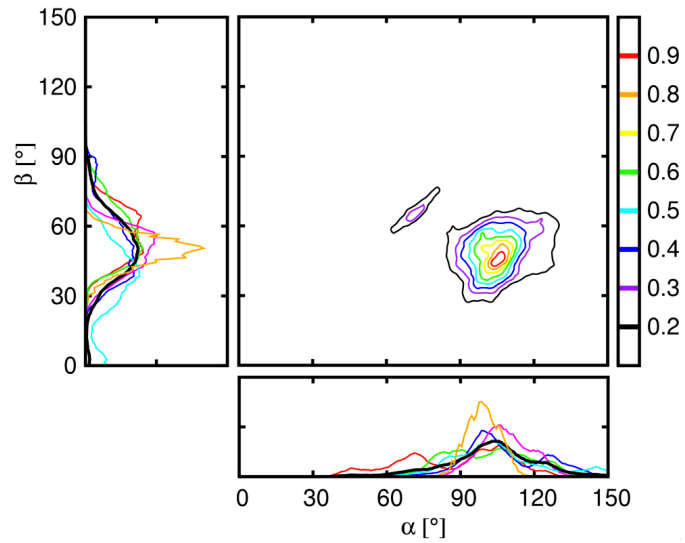


FIGURE S2. The average two-dimensional α and β distribution from all the multiple simulations shown as a contour map. The contour levels are indicated by different colors, and the color scale goes from black to red denoting population increase. The bottom and left panels show the distributions of α and β , respectively. The distributions from different systems are distinguished by colors with system cav1_45 in red, cav1_55 in green, cav1_65 in blue, cav1_75 in magenta, cav1_85 in cyan, and the 1- μ s simulation in orange. The averaged one-dimensional α and β distributions from the multiple simulations are in black.