Output Messages

Single TM helix:

Lowest energy helix-coil partition

Helix: 1 - 21, Stability: -20.2 (-13.9) kcal/mol

Helix 1: 1-21 LLLAFLLGLLLGTLLTVLILI

TM segments: 1(2-19)

transfer energy = -22.9 kcal/mol; thickness/depth = 31.2+-3.6 tilt = 37.+-5.

Aa seq. for dimer: LLLAFLLGLLLGTLLTVLILI

TM segment for dimer: 1 21

Model # 1 DGasc= -16.6 kcal/mol, DGstb= -16.9 kcal/mol, Easc= -32.0 kcal/mol, Rasym=0.0 A

Interhelix distance = 6.0 A, Angle = -46.

Key interfacial residues ():

LLLAFLL(G)LLL(G)TLLTVLILI

Model # 2 DGasc= -5.0 kcal/mol, DGstb= -17.6 kcal/mol, Easc= -25.3 kcal/mol, Rasym=0.2 A

Interhelix distance = 7.1 A, Angle = -29.

Key interfacial residues (): LLL(A)FLL(G)LLLGTLLTVLILI

Model # 3 DGasc= -5.3 kcal/mol, DGstb= -0.1 kcal/mol, Easc= -23.1 kcal/mol, Rasym=1.1 A

Interhelix distance = 8.3 A, Angle = -35.

Key interfacial residues (): LLLAFLLGLLL(G)TLL(T)VLILI

Model # 4 DGasc= -2.6 kcal/mol, DGstb= -11.5 kcal/mol, Easc= -21.6 kcal/mol, Rasym=0.5 A Interhelix distance = 8.6 A, Angle = 40.

Key helix-helix interface residues ():

LLLAF(L)LGLLLG(T)LLTVLILI

GLMOL Visualization

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GLMOL Visualization

Model 1

Model	ΔG_{asc}	ΔG_{stb}	Easc	Rasym	Distance	Angle
	kcal/mol	kcal/mol	kcal/mol	Å	Å	Degrees
1	-16.6	-16.9	-32.0	0.0	6.0	-46.0
2	-5.0	-17.6	-25.3	0.2	7.1	-29.0
3	-5.3	-0.1	-23.1	1.1	8.3	-35.0
4	-2.6	-11.5	-21.6	0.5	8.6	40.0

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