Output Messages

Single TM helix:

Lowest energy helix-coil partition

Helix: 1 - 21, Stability: -22.1 (-15.1) kcal/mol

Helix 1: 1-21 LLLSYLLVALLTLLLSFLILI

TM segments: 1(2-19)

transfer energy = -20.5 kcal/mol; thickness/depth = 31.2+-2.8 tilt = 29.+-23.

Aa seq. for dimer: LLLSYLLVALLTLLLSFLILI

TM segment for dimer: 1 21

Model # 1 DGasc= -8.6 kcal/mol, DGstb= -7.1 kcal/mol, Easc= -27.9 kcal/mol, Rasym=0.3 A Interhelix distance = 9.7 A, Angle = 25.

V av haliv haliv interfere residues ():

Key helix-helix interface residues ():

LLLS(Y)LL(V)ALL(T)LL(L)SFL(I)LI

Model # 2 DGasc= -8.8 kcal/mol, DGstb= -2.1 kcal/mol, Easc= -25.0 kcal/mol, Rasym=0.5 A Interhelix distance = 8.3 A, Angle = -41.

Key interfacial residues ():

LLLSYLL(V)ALL(T)LLLSFLILI

Model # 3 DGasc= -6.6 kcal/mol, DGstb= -1.2 kcal/mol, Easc= -21.6 kcal/mol, Rasym=0.8 A

Interhelix distance = 8.0 A, Angle = -27. Key interfacial residues ():

LLL(S)YLL(V)ALLTLLLSFLILI

Model # 4 DGasc= -5.3 kcal/mol, DGstb= -2.9 kcal/mol, Easc= -24.6 kcal/mol, Rasym=0.0 A

Interhelix distance = 8.0 A, Angle = 54.

Key helix-helix interface residues ():

LLLS(Y)LLVALL(T)LLLSFLILI

Model # 5 DGasc= -2.6 kcal/mol, DGstb= -6.6 kcal/mol, Easc= -20.1 kcal/mol, Rasym=0.6 A

Interhelix distance = 10.0 A, Angle = -7.

Key interfacial residues ():

LLL(S)YLL(V)AL(L)(T)LL(L)SFLILI

GLMOL Visualization

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GLMOL Visualization

Model 1 LLLSYLLVALLTLLLSFLILIY..V...T..L...I..

Model	ΔG_{asc}	ΔG_{stb}	Easc	Rasym	Distance	Angle	
	kcal/mol	kcal/mol	kcal/mol	Å	Å	Degrees	
1	-8.6	-7.1	-27.9	0.3	9.7	25.0	
2	-8.8	-2.1	-25.0	0.5	8.3	-41.0	
3	-6.6	-1.2	-21.6	0.8	8.0	-27.0	
4	-5.3	-2.9	-24.6	0.0	8.0	54.0	
5	-2.6	-6.6	-20.1	0.6	10.0	-7.0	

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