

Marqusee S, Baldwin RL. Helix stabilization by Glu-. . .Lys+ salt bridges in short peptides of de novo design. *Proc Natl Acad Sci.* **1987**; 84: 8898-8902

			-[θ]222	
i+4	E,K	A E A A A K E A A A K E A A A K A	29,000	helix content (pH 7.0, 1°C, 0.01 M NaCl)
i+4	K,E	A K A A A E K A A A E K A A A E A	25,300	
i+3	E,K	A E A A K A E A A K A E A A K A	17,600	
i+3	K,E	A K A A E A K A A E A K A A E A	8,500	

Huyghues-Despointes BM, Scholtz JM, Baldwin RL. Helical peptides with three pairs of Asp-Arg and Glu-Arg residues in different orientations and spacings. *Protein Sci.* **1993**; 2: 80-85

			-[θ]222	
i+4	D,R	A D A A A R D A A A R D A A A R Y	25,200	helix content (pH 7.0, 1°C, 0.01 M NaCl)
i+4	R,D	A R A A A D R A A A R D A A A R Y	16,300	
i+3	D,R	A D A A R A D A A R A D A A R Y	14,000	
i+3	R,D	A R A A D A R A A D A R A A D Y	2,200	
i+4	E,R	A E A A A R E A A A R E A A A R Y	31,300	
i+4	R,E	A R A A A E R A A A E R A A A E Y	22,400	
i+3	E,R	A E A A R A E A A R A E A A R Y	22,500	
i+3	R,E	A R A A E A R A A E A R A A E Y	11,800	

Scholtz JM, Qian H, Robbins VH, Baldwin RL. The energetics of ion-pair and hydrogen-bonding interactions in a helical peptide. *Biochemistry.* **1993**; 32: 9668-9676

			ΔG° (E ⁻ K ⁺)	ΔG° (E ⁰ K ⁺)	
i+4	Q,E	A A Q A A A E Q A A A A Q A A Y	-340	-380	Interactions (0.01 M NaCl)
i+4	Q,E	A A Q A A A A Q A A A E Q A A Y	-270	-300	
i+1	E,K	A A Q A E K A Q E A A A Q A A Y	200	0	
i+2	E,K	A A Q A E A K Q A A E A Q A A Y	180	-95	
i+3	E,K	A A Q A A E A Q K A A E Q A A Y	-380	-285	
i+4	E,K	A A Q A A E A Q A K A A Q E A Y	-470	-340	
i+3	K,E	A A Q A A K A Q E A A E Q A A Y	-460	-320	
i+4	K,E	A A Q A A K A Q A E A A Q E A Y	-380	-290	

Smith JS, Scholtz JM. Energetics of polar side-chain interactions in helical peptides: salt effects on ion pairs and hydrogen bonds. *Biochemistry.* **1998**; 37: 33/40

			-[θ]222	ΔG° (E ⁻ K ⁺)	
i+3	E,K	A A Q A A E A Q K A A A Q A A Y	11,400	-290	helix content (0°C, 0.01 M NaCl, pH 5.5/7.0)
i+4	E,K	A A Q A A E A Q A K A A Q A A Y	12,750	-415	
i+5	E,K	A A Q A A E A Q A A K A Q A A Y	8,500		
i+3	K,E	A A Q A A K A Q E A A A Q A A Y	9,000	-280	
i+4	K,E	A A Q A A K A Q A E A A Q A A Y	10,350	-400	
i+5	K,E	A A Q A A K A Q A A E A Q E A Y	6,900		
i+3	D,K	A A Q A A D A Q K A A A Q A A Y	8,200	-120	
i+4	D,K	A A Q A A D A Q A K A A Q A A Y	9,200	-240	
i+5	D,K	A A Q A A D A Q A A K A Q A A Y	7,400		
i+3	K,D	A A Q A A K A Q D A A A Q A A Y	8,400	-400	
i+4	K,D	A A Q A A K A Q A D A A Q A A Y	10,300	-580	
i+5	K,D	A A Q A A K A Q A A D A Q E A Y	5,800		
i+3	E,H	A A Q A A E A Q H A A A Q A A Y	4,500	-300	
i+4	E,H	A A Q A A E A Q A H A A Q A A Y	4,100	-190	
i+5	E,H	A A Q A A E A Q A A H A Q A A Y	3,600		
i+3	H,E	A A Q A A H A Q E A A A Q A A Y	4,400	-500	
i+4	H,E	A A Q A A H A Q A E A A Q A A Y	5,300	-650	
i+5	H,E	A A Q A A H A Q A A E A Q E A Y	2,300		

Waggawagga scoring

Stabilization / destabilization by amino acid interactions

Source residue	Target residue	Interaction	Score	Stabilization
H/K/R	E	i+4	1.0	strong
E	K/R	i+4	1.0	strong
H/K/R	E	i+3	0.75	medium
E	K/R	i+3	0.75	medium
K/R	D	i+4	0.75	medium
K/R	D	i+3	0.5	weak
D	K/R	i+4	0.75	medium
D	K/R	i+3	0.5	weak
E	H	i+3	0.5	weak
Q	E	i+4; i+3	0.5	weak
E	Q	i+4; i+3	0.5	weak
network stabilization (oppositely charged residues)		i, i+3, i+6	1.5	network
		i, i+3, i+7	0.25	network
		i, i+4, i+7	0.25	network
		i, i+4, i+8	2.0	network
hydrophobic seam		i, i+3, i+6	-0.5	destabilizing
		i, i+3, i+7	-0.5	destabilizing
		i, i+4, i+7	-0.5	destabilizing
		i, i+4, i+8	-0.5	destabilizing

Stabilization / destabilization by helix-forming propensity

Residue	Score	Stabilization
A	0.25	stabilizing
G	-0.5	destabilizing
P	-0.75	destabilizing