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Supplemental Information

Binding Mechanism of the N-Terminal SH3 Domain of CrkII and Proline-Rich Motifs in cAbl

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Table S1. Proline-rich motifs (PRMs) in human cAbl-1A tested for the binding to the nSH3 domain of CrkII

Sequence[a]	K_d (μM)
PRM^{524} QA**P**ELPTKTRTSY	1.72 ± 0.47
PRM^{546} DV**P**EMPHSKGQY	N. D.
PRM^{568} VS**P**LLPRKERGY	2.90 ± 0.19
PRM^{610} TA**P**TPPKRSSSY	N. D.
PRM^{758} YEK**P**ALPRKR	1.72 ± 0.48
PRM^{781} YR**P**PPRLVKK	N. D.
PRM^{897} PA**P**PPPPAASAY	N. D.
PRM^{956} KK**P**VLPATPKPQY	N. D.

[a] The number in the peptide name corresponds to the amino acid number of first proline in each sequence (shown in bold). Tyrosine is added to either the N- or the C-terminal end of each peptide to measure the concentration of the peptide.

Table S2. Data Collection and Refinement Statistics

	Data Collection
source	Cu Kα
space group	$P12_11$
unit cell parameters	
a, b, c (Å)	45.2, 29.5, 45.8
α, β, γ (deg)	90.0, 94.3, 90.0
temperature (K)	113.15
wavelength (Å)	1.5
resolution (Å)	50.00-1.80 (1.83-
R_{merge}[b]	0.14 (0.17)
completeness (%)	99.1 (98.9)
$\langle I/\sigma(I)\rangle$	38.1 (27.6)
total number of reflections	39207
Average redundancy	3.5 (3.3)
	Refinement Statistics
resolution (Å)	45.6-1.8
number of reflections	10714
R_{factor}[c]	0.17
R_{free}[c]	0.24
number of protein atoms per chain	501
number of water atoms	181
number of ligand atoms per chain	94
rms deviation from ideal values[d] for bond distances	0.022
rms deviation from ideal values for bond angles	2.04
average B-factors	
chain A of the protein (Å^2)	17.80
chain B of the protein (Å^2)	19.60
chain M of the ligand (Å^2)	30.00
chain N of the ligand (Å^2)	24.60
water molecules (Å^2)	31.11
Ramachandran plot[e]	
favored (%)	98.32
disallowed (%)	0

[a]The numbers in parentheses refer to the highest resolution shell.

[b]$R_{merge} = \sum_{hkl} \sum_j |I_{hkl,j} - \langle I_{hkl}\rangle| / \sum_{hkl} \sum_j \langle I_{hkl}\rangle$

[c]$R_{factor} = \sum|F_{obs}-F_{calc}|/\sum|F|_{obs}$, where R_{free} refers to the R_{factor} for 5% of the data that

[d]Ideal values used from Engh and Huber (1)

[e]Validation by COOT (2)

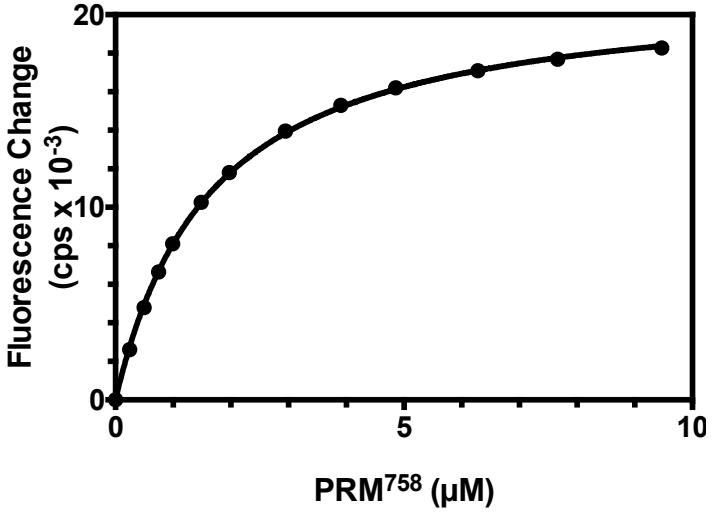

Figure S1. Binding isotherm of PRM^{758} to the nSH3 domain at pH 7.5 in Hepes buffer. The measured K_d is 1.6 μM.

Supporting References

1. Engh, R. A., and R. Huber. 1991. Accurate bond and angle parameters for X-ray protein structure refinement. Acta Crystallogr A 47:392-400.
2. Emsley, P., and K. Cowtan. 2004. Coot: model-building tools for molecular graphics. Acta Crystallogr D Biol Crystallogr 60:2126-2132.