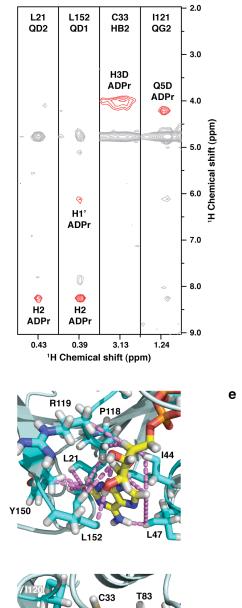
## **Supplementary Data**

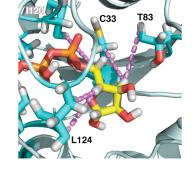
## ORPHAN MACRODOMAIN (HUMAN C6ORF130) IS AN *O*-ACYL-ADP-RIBOSE DEACYLASE: SOLUTION STRUCTURE AND CATALYTIC PROPERTIES Francis C. Peterson<sup>1§</sup>, Dawei Chen<sup>1¶</sup>, Betsy L. Lytle<sup>1§</sup>, Marianna N. Rossi<sup>#</sup>, Ivan Ahel<sup>#</sup>, John M. Denu<sup>2¶</sup>, and Brian F. Volkman<sup>2§</sup>

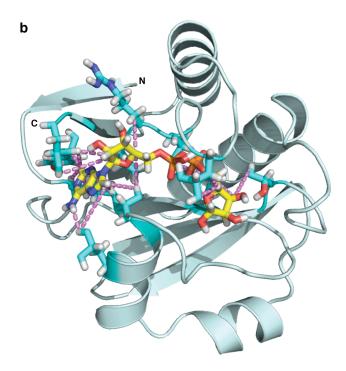


С

d







)	Residue	Residue atom	ADPr atom	Residue	Residue atom	ADPr atom
	L21	Н	H2	R119	HB2	H4'
	L21	HA	H2	R119	HB3	H4'
	L21	HB2	H2	R119	QB	H4'
	L21	HB3	H2	1120	QG2	Q5D
	L21	QB	H2	L124	HB2	H4D
	L21	QD1	H2	L124	HB3	H4D
	L21	QD2	H2	L124	QQD	H4D
	L21	QQD	H2	Y150	HB2	H2
	C33	QB	H3D	Y150	HB3	H2
	144	HB	H8	Y150	QB	H2
	144	QD1	H2	L152	н	H2
	144	QD1	H8	L152	HG	H2
	144	QG2	H4'	L152	QD1	H1'
	144	QG2	H8	L152	QD1	H2
	L47	QQD	H8	L152	QD2	H1'
	L47	QQD	Q6	L152	QD2	H2
	T83	QG2	H3D	L152	QQD	H1'
	P118	HA	H2	L152	QQD	H2
	P118	HB2	H4'	L152	QQD	H8
	P118	HB3	H4'			

**Figure S1. Intermolecular NOE contacts defining the C6orf130:ADPr complex.** (a) Representative strips from the 3D <sup>13</sup>C-edited/<sup>13</sup>C-filtered NOESY spectrum containing intermolecular NOE crosspeaks. (b) Overview of the bound ADPr ligand with NOE distance constraints. Close-up views of the adenosine and promixal ribose (c) and distal ribose (d) with intermolecular NOE constraints. (e) All intermolecular NOEs used to solve the structure are listed.

Proteins SAV0325	C6orf130 <sup><i>a</i></sup>	MacroD1 <sup>b</sup>	MacroD2	<i>E. coli</i> YmdB	S. aureus
C6orf130		19.7 <sup>c</sup>	19.1	17.8	21.7
macroD1			61.1	47.2	38.5
macroD2				49.7	32.3
E. coli YmdB					40.7
S. aureus SAV0325					

## Table S1. Sequence comparison of C6orf130 protein with macro family proteins

<sup>a</sup>Mungall, A. J. et al. (2003) Nature **425**, 805-811.

<sup>b</sup>Chen, D. et al. (2011) *J. Biol. Chem.* **286**, 13261-13271 <sup>c</sup>Numbers indicate percentage of sequence identity between the overlapping region of the two sequences compared.