Supporting Information

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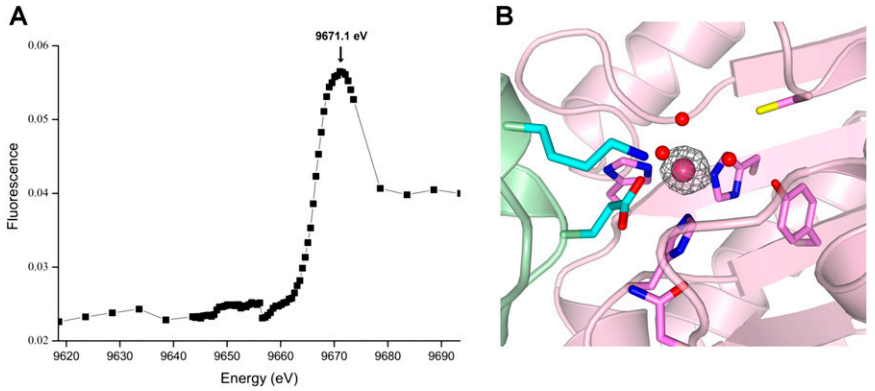

Fig. S1. Presence of a zinc ion in the active site. (*A*) X-ray fluorescence spectrum of 5-methylthioribulose-1-phosphate dehydratase/Apaf-1 interacting protein (MtnB/APIP) crystal around a zinc absorption edge. (*B*) Anomalous difference map is contoured at the level of 5 σ cutoff. The diffraction data are collected at the wavelength corresponding to the peak in *A*, 1.28201 Å. The view is same as in Fig. 3*A*.

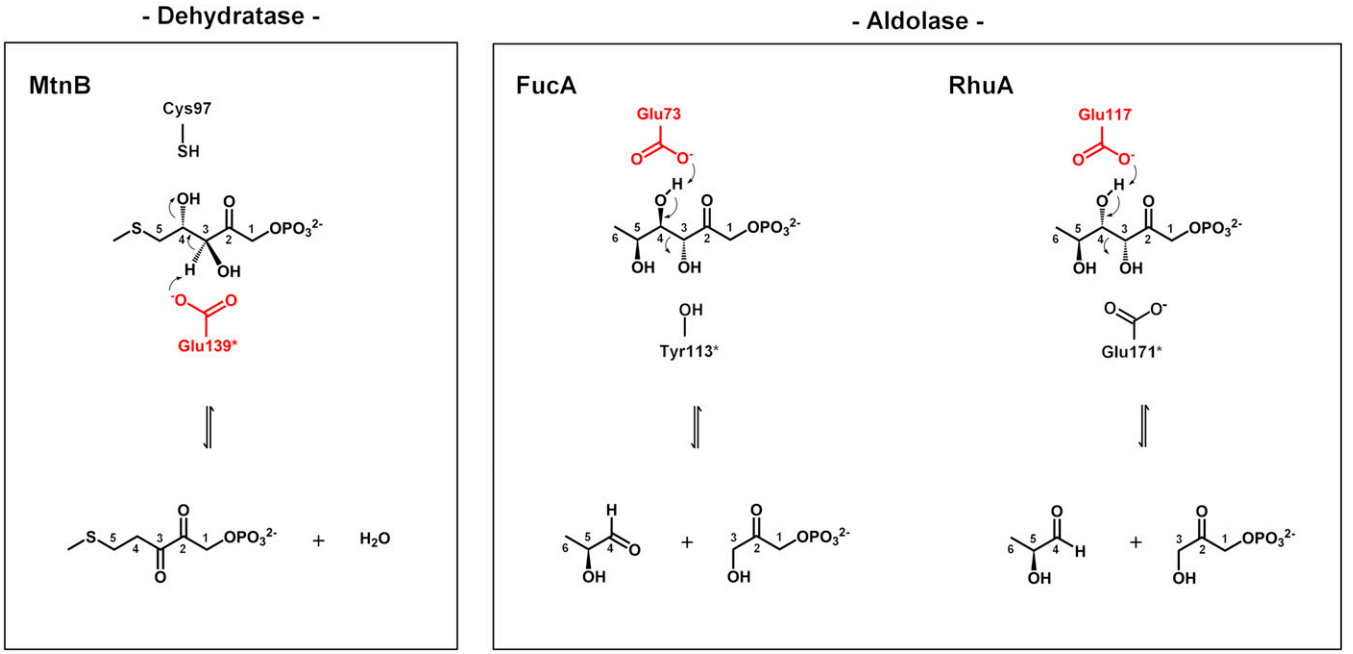

Fig. S2. Biochemical features of APIP/MtnB as a dehydratase contrasting to aldolases such as FucA and RhuA. Dehydration reaction by APIP/MtnB does not involve C-C bond cleavage, which is characteristic of the aldolase reactions. The catalytic acid/base residue of APIP/MtnB is located at the opposite side of the substrate in comparison with aldolases; Glu139* of APIP/MtnB is located at the C3-side of the substrate, but Glu73 of FucA and Glu117 of RhuA commonly at the C4-side of the corresponding substrates. Connectedly, the initial proton abstraction occurs at C3 in APIP/MtnB's dehydratase reaction, but it occurs, in contrast, at O4 in aldolase reactions by FucA and RhuA.

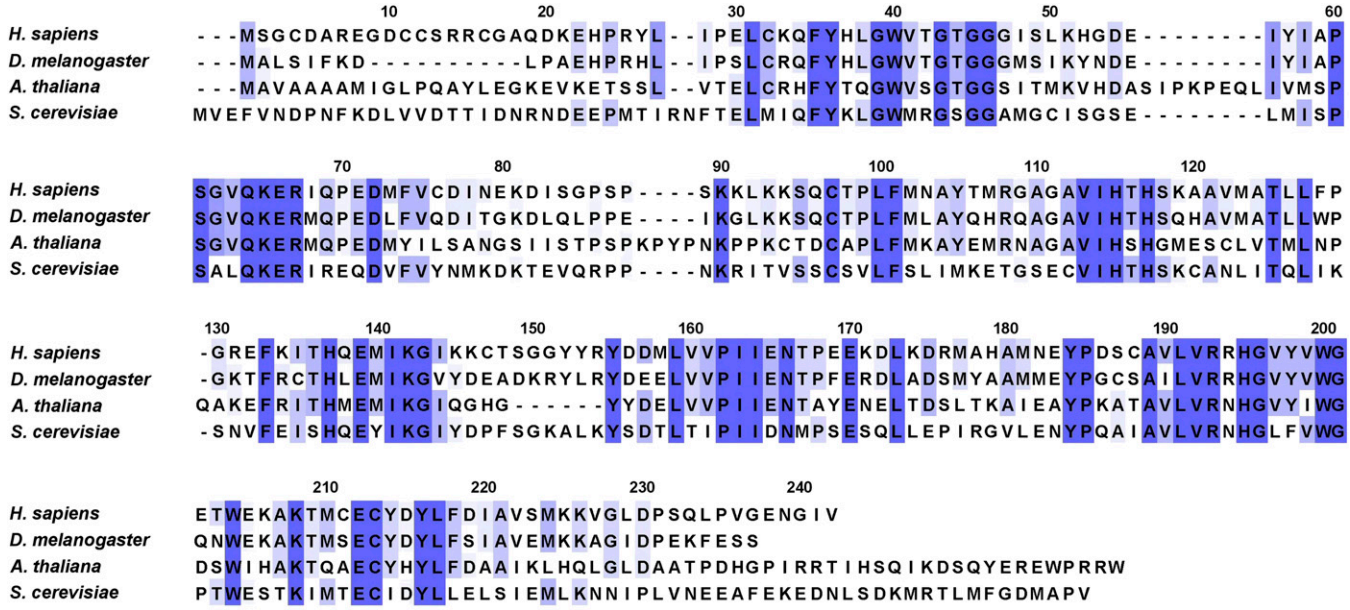

Fig. S3. Sequence conservation of APIP/MtnB through multicellular organisms. APIP/MtnB sequences from four multicellular organisms are aligned. Conserved residues are boxed in blue.

Table S1. Summary of structure determination and refinement

Data collection					
Data set		Br soaked			Native
Space group		$C222_1$			$C222_1$
Wavelength, Å	Edge, 0.91977	Peak, 0.91957	Remote, 0.90633	1.00000	1.28201 (zinc edge)
Unit cell, Å	a = 106.81	a = 106.78	a = 106.83	a = 107.04	a = 107.10
	b = 107.29	b = 107.27	b = 107.30	b = 107.74	b = 107.76
	c = 191.06	c = 191.00	c = 191.09	c = 192.10	c = 190.92
Resolution, Å	30.00–2.20	30.00–2.20	30.00–2.20	50.00–2.00	30.00–2.30
Reflections, total/unique	658,243/54,020	655,403/53,922	659,382/54,053	458,706/72,069	528,270/46,689
Completeness, %	95.8 (75.3)	95.7 (74.6)	95.7 (74.8)	96.0 (81.2)	95.0 (93.1)
R_{merge}, %	4.8 (16.9)	4.3 (15.7)	4.8 (17.1)	6.4 (37.8)	13.6 (25.5)
Redundancy	12.2 (6.7)	12.2 (6.7)	12.2 (6.5)	6.4 (5.0)	11.3 (11.4)
$\langle I \rangle / \langle \sigma(I) \rangle$	64.6 (13.1)	63.7 (13.0)	62.7 (12.4)	31.2 (4.1)	13.9 (7.4)
Phasing					
Br sites	10				
Figure of merit	0.405 from SOLVE/0.709 from RESOLVE				
Model refinement					
R_{work}/R_{free}, %				18.3/22.0	15.6/19.8
RMS deviation in bond lengths/angles, Å/°				0.026/2.049	0.019/2.011
Number of nonhydrogen atoms/average B-factor, Å^2					
Protein (893 residues for four subunits)				7053/30.0	7053/31.7
Zinc				4/18.9	4/26.4
Water				567/37.1	567/37.9
Ramachandran plot, no. of residues (%)					
In preferred region				857 (96.84)	844 (95.37)
In allowed region				25 (2.82)	35 (3.95)
Outliers				3 (0.34)	6 (0.68)

Values in parentheses are for the highest-resolution shell; 2.24–2.20 Å for Br-MAD data sets, 2.07–2.00 Å for the native data set at 1.00000 Å, and 2.42–2.30 Å for the native data set at 1.28201 Å.