

# Mechanistic and Evolutionary Insights from the Reciprocal Promiscuity of Two Pyridoxal Phosphate-Dependent Enzymes

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## SUPPLEMENTAL TABLES

**Table S1.** Days to form colonies for various *E. coli* strains grown on M9/glucose medium, supplemented with IPTG (50  $\mu$ M).

Over-expressed protein	$\Delta metC$	$\Delta metC$ + L-methionine	$\Delta metE$	$\Delta metE$ + L-methionine
CBL	1–2	1–2	NT*	NT*
None (empty vector)	No growth	1–2	No growth	2
ALR-GFP	5–6	NT*	NT*	NT*
ALR	3–4	1–2	No growth	2
Methionine synthase	NT*	NT*	2	2

\*NT: Not tested.

**Table S2.** Crystal properties, data collection and refinement statistics.

	ALR(Y274F)	ALR(Y274F) + L-Ala-P	CBL(P113S)	CBL(P113S) + L-Ala-P
<b>PDB entry</b>	4WR3	4XBJ	4ITG	4ITX
<b>Data collection</b>				
Space group	<i>P6</i>	<i>P6</i>	<i>C222</i> <sub>1</sub>	<i>C222</i> <sub>1</sub>
Unit-cell parameters:				
<i>a</i> (Å)	148.08	147.98	59.93	59.97
<i>b</i> (Å)	148.08	147.98	152.77	153.22
<i>c</i> (Å)	163.69	163.58	150.85	150.91
$\alpha, \beta, \gamma$ (°)	90, 90, 120	90, 90, 120	90, 90, 90	90, 90, 90
Beamline	Rotating anode	Rotating anode	Rotating anode	Rotating anode
Resolution	1.86 (1.90-1.86)	2.25 (2.29-2.25)	1.74 (1.83-1.74)	1.61 (1.69-1.61)
Wavelength (Å)	1.5418	1.5418	1.5418	1.5418
CC <sub>1/2</sub>	0.998 (0.632)	0.992 (0.617)	1.000 (0.976)	1.000 (0.881)
Completeness (%)	99.6 (93.8)	99.7 (97.0)	99.7 (98.3)	99.0 (93.7)
Observed reflections	168,143	95,615	71,753	89,828
$\langle I/\sigma(I) \rangle$	18.5 (1.9)	10.7 (2.0)	35.7 (8.7)	25.6 (4.2)
Multiplicity	22.1 (16.4)	11.4 (10.2)	15.9 (14.8)	11.6 (9.7)
<b>Refinement</b>				
Resolution range	19.7-1.90	19.9-2.25	19.5-1.74	76.6-1.61
Reflections used	149,471	90,731	67,348	85,255
<i>R</i> factor	0.175	0.167	0.164	0.164
<i>R</i> <sub>free</sub>	0.204	0.202	0.203	0.199
Average <i>B</i> factor (Å <sup>2</sup> )	22.8	21.7	16.5	16.2
RMS deviation from ideal:				
Bond lengths (Å)	0.008	0.008	0.020	0.022
Bond angles (°)	1.349	1.142	2.126	2.157
Ramachandran plot (%):				
Favoured	96.8	96.2	97.2	97.8
Outliers	0.0	0.0	0.0	0.0
Molprobrity server score	93 <sup>rd</sup> percentile	96 <sup>th</sup> percentile	93 <sup>rd</sup> percentile	94 <sup>th</sup> percentile

Data for the high resolution shell are shown in parentheses.

## SUPPLEMENTAL FIGURE

**Figure S1.** 2Fo – Fc electron density maps of the PLP sites in ALR(Y274F), ALR(Y27F)–L-Ala-P, CBL(P113S) and CBL(P113S)–L-Ala-P. Each map is contoured at 1 $\sigma$ .

