

## SUPPORTING INFORMATION

# Crystal Structure of Aldehyde Dehydrogenase 16 Reveals Trans Hierarchical Structural Similarity and a New Dimer

Li-Kai Liu<sup>1</sup> and John J. Tanner<sup>1,2</sup>

Departments of <sup>1</sup>Biochemistry and <sup>2</sup>Chemistry, University of Missouri, Columbia, Missouri 65211, USA

Corresponding author: John J. Tanner, Department of Biochemistry, University of Missouri, Columbia, MO 65211, USA. Tel: (573) 884-1280; Email: [tannerjj@missouri.edu](mailto:tannerjj@missouri.edu).

### Table of Contents

---

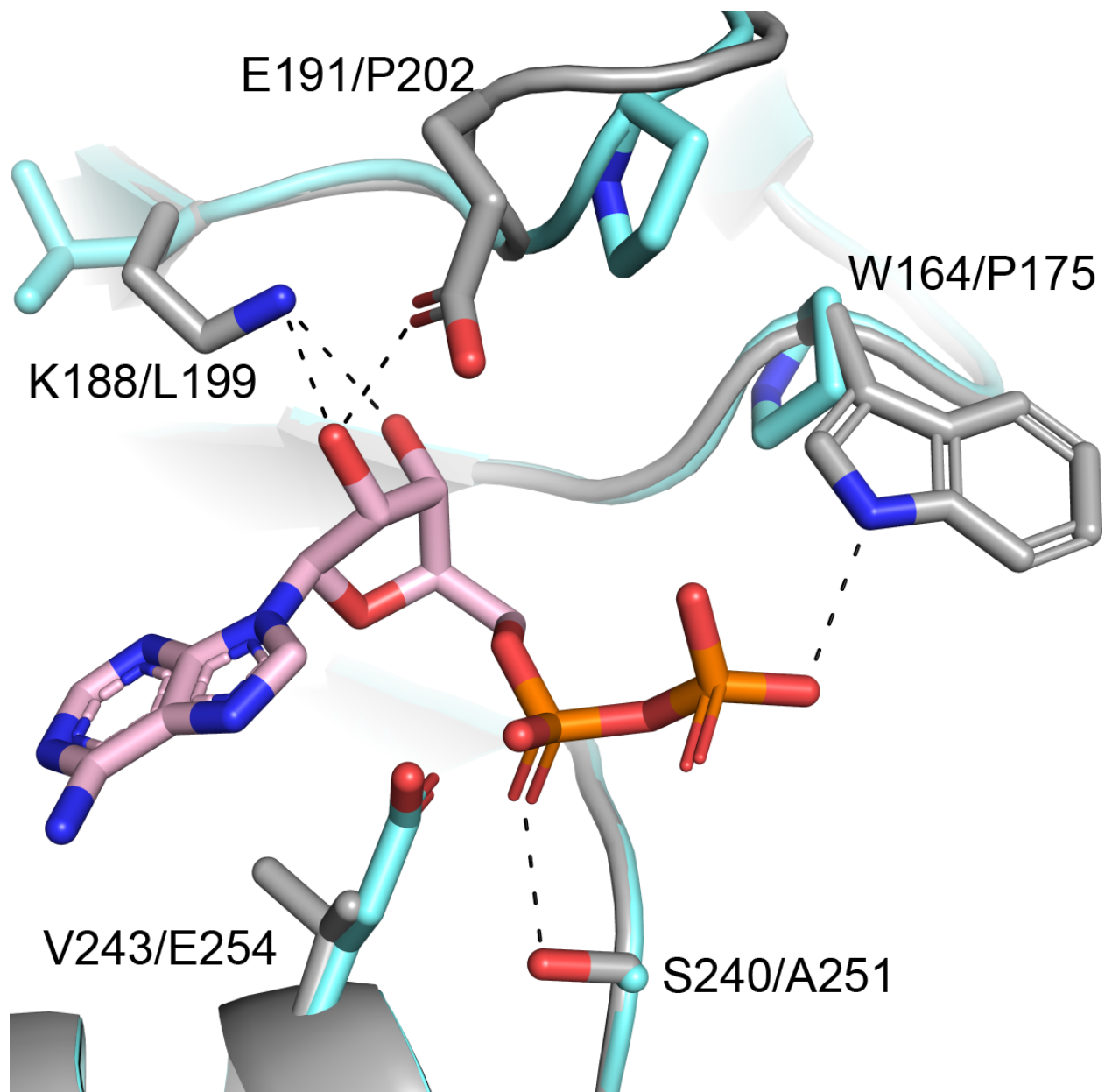
Table S1. Data Collection Statistics for LaALDH16.....	S-2
Fig. S1. Model of the nonfunctional NAD <sup>+</sup> -binding site of HsALDH16A1 .....	S-3
Fig. S2. Catalytic activity of ALDH16 .....	S-4

---

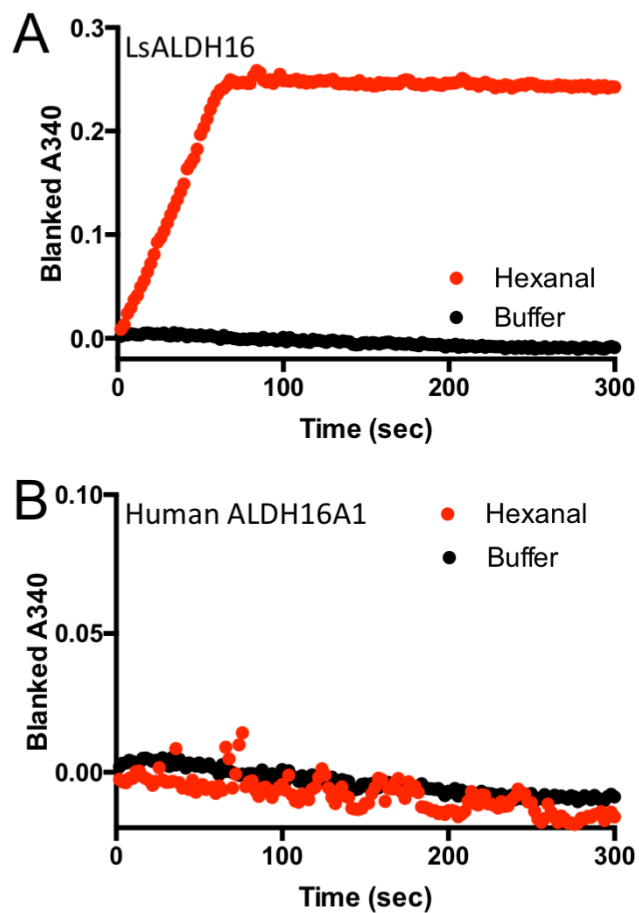
**Table S1.** Data Collection Statistics for LaALDH16<sup>a</sup>

Beamline	ALS 4.2.2
Space group	<i>P2</i>
Unit cell parameters (Å, °)	<i>a</i> = 97.9, <i>b</i> = 63.1, <i>c</i> = 134.1, $\beta$ = 108.9°
Wavelength (Å)	1.000
Resolution (Å)	63.08-2.95 (3.11-2.95)
Observations	116172 (15801)
Unique reflections	32443 (4706)
$R_{\text{merge}}(I)$	0.088 (0.627)
$R_{\text{meas}}(I)$	0.122 (0.856)
$R_{\text{pim}}(I)$	0.083 (0.580)
Mean $I/\sigma$	10.5 (1.7)
Mean $CC_{1/2}$	0.996 (0.631)
Completeness (%)	98.4 (98.6)
Multiplicity	3.6 (3.4)

<sup>a</sup>Values for the outer resolution shell of data are given in parentheses.



**Fig. S1.** Model of the nonfunctional NAD<sup>+</sup>-binding site of HsALDH16A1. This figure shows a superposition of the crystal structure of LsALDH16-NAD<sup>+</sup> (gray with pink NAD<sup>+</sup>) and a model of HsALDH16A1 generated with SWISS-MODEL (blue). Residues are labeled as LsALDH16/HsALDH16A1.



**Fig. S2.** Catalytic activity of ALDH16 monitored by the progress curve of NADH production using hexanal as the substrate in the presence of the cofactor  $\text{NAD}^+$ . (A) LsALDH16 displays ALDH activity. (B) HsALDH16A1 does not display ALDH activity.