# SUPPORTING INFORMATION

# Ligand-dependent dynamics of the active-site lid in bacterial dimethylarginine dimethylaminohydrolase

Masooma Rasheed<sup>†</sup>, Christine Richter<sup>†</sup>, Liisa T. Chisty<sup>‡</sup>, John Kirkpatrick<sup>§</sup>, Martin Blackledge<sup>¶</sup>, Martin R. Webb<sup>‡</sup>, and Paul C. Driscoll<sup>†</sup>,<sup>\*</sup>

†Division of Molecular Structure, MRC National Institute for Medical Research, The Ridgeway, Mill Hill, London NW7 1AA, United Kingdom

Division of Physical Biochemistry, MRC National Institute for Medical Research, The Ridgeway, Mill Hill, London NW7 1AA, United Kingdom

§Institute of Structural and Molecular Biology, Division of Biosciences, University College London, Gower Street, London WC1E 6BT, United Kingdom

Protein Dynamics and Flexibility, Institut de Biologie Structurale, CEA, CNRS, UJF-Grenoble 1, 41 Rue Jules Horowitz, F-38027 Grenoble, France

#### AUTHOR INFORMATION

#### **Corresponding Author**

\*P. C. Driscoll. E-mail: pdrisco@nimr.mrc.ac.uk. Phone: +44 (0)20 8816 2061. Fax: +44 (0)20 8906 4477.



### **Supplementary Figure 1**

<sup>15</sup>N nuclear relaxation measurements for *apo* TM-PaDDAH. Per-residue <sup>15</sup>N R<sub>1</sub>, <sup>15</sup>N R<sub>2</sub> and  $\{^{1}H\}^{15}N$  heteronuclear NOE (hNOE) values obtained at <sup>1</sup>H 600MHz (blue) and 800 MHz (red) and 25°C. The secondary structure of PaDDAH is depicted at the top of the figure.



# **Supplementary Figure 2**

<sup>15</sup>N nuclear relaxation measurements for L-citrulline-saturated TM-PaDDAH. Per-residue <sup>15</sup>N R<sub>1</sub>, <sup>15</sup>N R<sub>2</sub> and {<sup>1</sup>H}<sup>15</sup>N heteronuclear NOE (hNOE) values obtained at <sup>1</sup>H 600MHz (blue) and 800 MHz (red) and 25°C. The secondary structure of PaDDAH is depicted at the top of the figure.



## **Supplementary Figure 3**

Representative time-resolved stopped-flow fluorescence traces obtained by mixing of 2.5  $\mu$ M S20C-MDCC-labeled DM-PaDDAH (*fl*-DM-PaDDAH) with ADMA at the indicated concentrations.