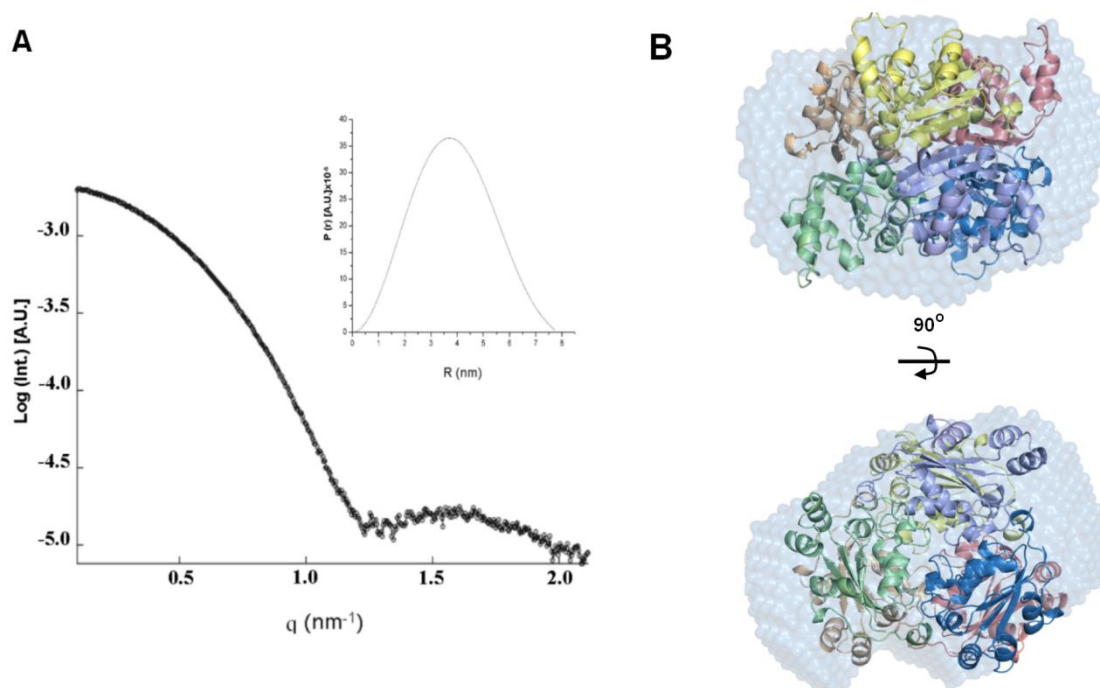


## ELETRONIC SUPPLEMENTARY INFORMATION

### Molecular adaptability of nucleoside diphosphate kinase b from trypanosomatid parasites: Stability, oligomerization and structural determinants of nucleotide binding

Tatiana A.C.B. Souza<sup>1,#</sup>, Daniel M. Trindade<sup>1,#</sup>, Celisa C.C. Tonoli<sup>1</sup>, Camila R. Santos<sup>1</sup>, Richard J. Ward<sup>2</sup>, Raghuvir K. Arni<sup>3</sup>, Arthur H.C. Oliveira<sup>2</sup> & Mário T. Murakami<sup>1,\*</sup>

**Figure S1:** Oligomerization of LmNDKb. Experimental scattering curve (A) and the pair-distance distribution function  $p(r)$  (inset, Fig. S1A). (B) Crystallographic hexamer fitted into the SAXS envelope.



**Suppl. Table 1:** Interactions between LmNDKb residues and ligands.

Ligand	Distance (Å)	LmNDK + PO <sub>4</sub> Form I
PO <sub>4</sub> <sup>(1)</sup> O4	2.36	His <sup>117A</sup> N <sup>D1</sup>
PO <sub>4</sub> <sup>(1)</sup> O1	3.12	Arg <sup>87A</sup> N <sup>H2</sup>
PO <sub>4</sub> <sup>(1)</sup> O3	2.63	Arg <sup>87A</sup> N <sup>H2</sup>
PO <sub>4</sub> <sup>(1)</sup> O3	3.37	Arg <sup>104A</sup> N <sup>H2</sup>
<b>LmNDKb + PO<sub>4</sub> Form II</b>		
PO <sub>4</sub> <sup>(1)</sup> O <sup>2</sup>	2.85	Lys <sup>11A</sup> N <sup>Z</sup>
PO <sub>4</sub> <sup>(1)</sup> O <sup>4</sup>	2.91	His <sup>117A</sup> N <sup>D1</sup>
PO <sub>4</sub> <sup>(2)</sup> O <sup>1</sup>	2.94	Arg <sup>104A</sup> N <sup>H1</sup>
PO <sub>4</sub> <sup>(2)</sup> O <sup>2</sup>	2.66	Arg <sup>104A</sup> N <sup>H2</sup>
PO <sub>4</sub> <sup>(2)</sup> O <sup>4</sup>	2.93	Arg <sup>87A</sup> N <sup>H2</sup>
PO <sub>4</sub> <sup>(2)</sup> O <sup>4</sup>	2.71	Arg <sup>87A</sup> N <sup>E</sup>
PO <sub>4</sub> <sup>(2)</sup> O <sup>4</sup>	3.70	His <sup>117A</sup> N <sup>D1</sup>
PO <sub>4</sub> <sup>(3)</sup> O <sup>1</sup>	2.90	His <sup>117C</sup> N <sup>D1</sup>
PO <sub>4</sub> <sup>(3)</sup> O <sup>1</sup>	2.52	Lys <sup>11C</sup> N <sup>Z</sup>
DTT <sup>(1)</sup> SA	3.17	Arg <sup>87B</sup> N <sup>H1</sup>
DTT <sup>(1)</sup> O <sup>2</sup>	3.10	Lys <sup>11B</sup> N <sup>Z</sup>
DTT <sup>(1)</sup> O <sup>2</sup>	3.04	Asn <sup>114B</sup> N <sup>D2</sup>
DTT <sup>(1)</sup> O <sup>3</sup>	2.81	His <sup>117B</sup> N <sup>D1</sup>
<b>LmNDKB + AMP</b>		
AMP-O1P	2.67	Lys <sup>11</sup> N <sup>Z</sup>
AMP-O1P	2.79	His <sup>117</sup> N <sup>D1</sup>
AMP-O3P	3.10	Asn <sup>114</sup> N <sup>D2</sup>
AMP-O3P	2.95	Tyr <sup>51</sup> O <sup>H</sup>
AMP-O3P	2.97	Lys <sup>11</sup> N <sup>Z</sup>
<b>LmNDK + ADP</b>		
ADP-O1P	2.80	Arg <sup>87</sup> N <sup>H1</sup>
ADP-O2P	2.70	Thr <sup>93</sup> O <sup>G1</sup>
ADP-O2P	2.98	Arg <sup>104</sup> N <sup>H1</sup>
ADP-O2P	2.91	Arg <sup>87</sup> N <sup>H1</sup>
ADP-O3P	3.11	Arg <sup>104</sup> N <sup>H2</sup>
ADP-O3*	2.85	Asn <sup>114</sup> N <sup>D2</sup>
ADP-O3*	2.77	Lys <sup>11</sup> N <sup>Z</sup>
ADP-O2*	3.08	Lys <sup>11</sup> N <sup>Z</sup>