Simulation of kinetic data shown in Figure 1A

The velocity equation 1 was transformed into a computer readable formula \( f(a) \) where \( f \) is velocity measured and \( a \) the total ATP concentration used. The formula is:

\[
f = \frac{(((m+a+k0)/2-(((m+a+k0)/2)^2)-m*a)^.5)/k1)}{(((m+a+k0)/2-(((m+a+k0)/2)^2)-m*a)^.5)*k2+((((m+a+k0)/2-(((m+a+k0)/2)^2)-m*a)^.5)/k3)}
\]

Parameters \( m \) (total Mg concentration), \( k1 \) (K1), \( k2 \) (K1') and \( k3 \) (KMg) were constrained according to the series and the values from the double reciprocal analysis in Table 2 and the data using a nonlinear regression program (SigmaPlot 2001).
Equation 1:

\[
V = \frac{[MgATP] \cdot V_{\text{max}} + [Mg][MgATP] \cdot V'_{\text{max}}}{K_1 + \frac{[Mg]}{K_{Mg}} + \frac{[MgATP]}{K_i} + \frac{[Mg][MgATP]}{K_{Mg} \cdot K_i'}}
\]

or in terms of \([Mg]_{\text{total}}\) and \([ATP]_{\text{total}}\) replace:

\[
[MgATP] = \frac{[Mg]_{\text{total}} + [ATP]_{\text{total}} + Ko}{2} - \sqrt{\left(\frac{[Mg]_{\text{total}} + [ATP]_{\text{total}} + Ko}{2}\right)^2 - [Mg]_{\text{total}} \cdot [ATP]_{\text{total}}}
\]

\[
[Mg] = [Mg]_{\text{total}} - \frac{[Mg]_{\text{total}} + [ATP]_{\text{total}} + Ko}{2} - \sqrt{\left(\frac{[Mg]_{\text{total}} + [ATP]_{\text{total}} + Ko}{2}\right)^2 - [Mg]_{\text{total}} \cdot [ATP]_{\text{total}}}
\]

where \(Ko = K_d(MgATP)\)