



STRUCTURAL
BIOLOGY

Volume 77 (2021)

Supporting information for article:

X-ray diffraction and *in vivo* studies reveal the quinary structure of *Trypanosoma cruzi* nucleoside diphosphate kinase 1: a novel helical oligomer structure

Juan Arturo Gomez Barroso, Mariana Reneé Miranda, Claudio Alejandro Pereira, Richard Charles Garratt and Carlos Fernando Aguilar

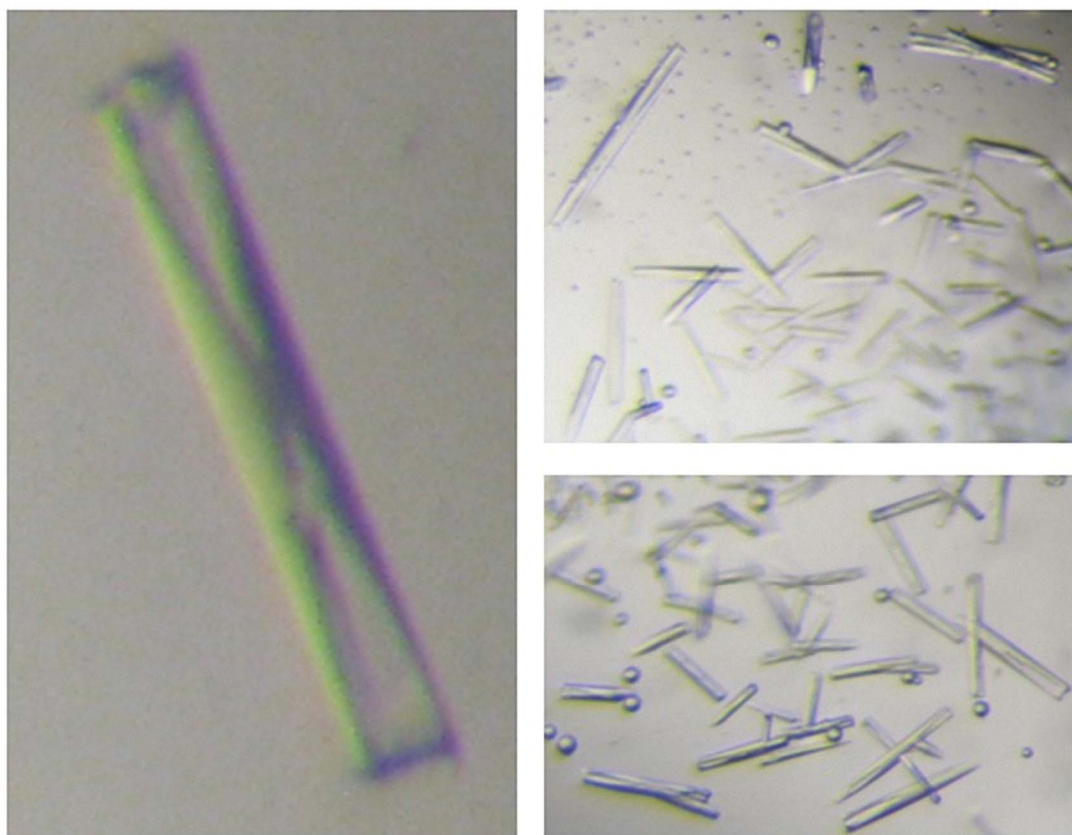


Figure S1 TcNDPK1 Crystals. The figure shows TcNDPK1 crystals obtained in the condition described in the methods section. Note the rod like shape.

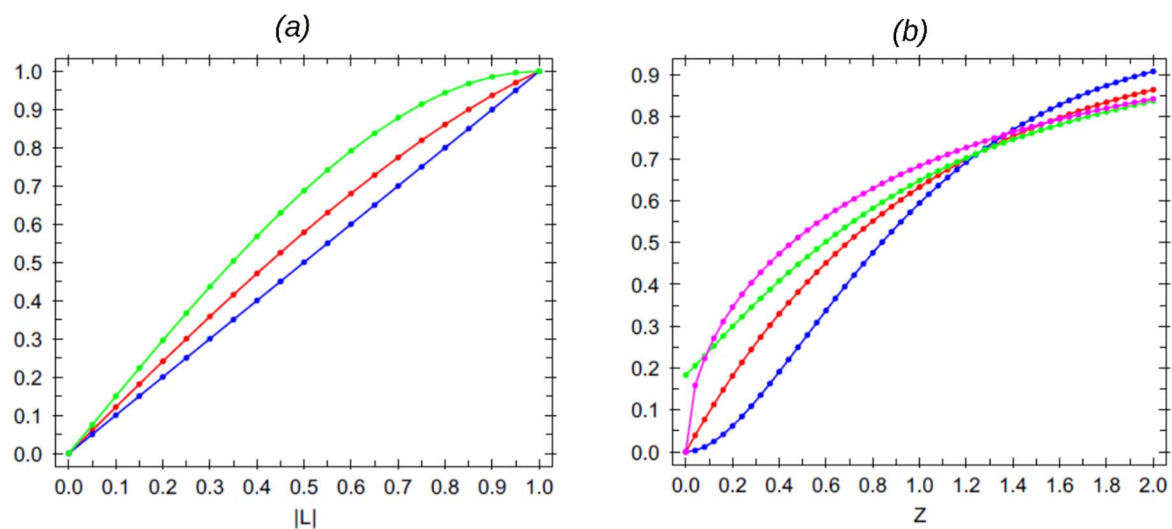


Figure S2 Twin analysis (a) The cumulative distribution for the L-test showed similar values to the expected curve for untwinned data. Untwinned (blue), observed (red) and twinned (green). The L-test gave a twinning fraction of 0.11. (b) The cumulative intensity statistics distribution (Z plot), is a test to estimate twin fractions from tetartohedral twinned data. The Z plot for tetartohedral twinned intensities has a sigmoidal shape (blue). The theoretical values have an exponential curve (red). The observed values are showed in green, and had an exponential shape that would correspond to untwinned intensities.

(a)

```

--- Peaks of Rotation Function ---
+-----+-----+-----+-----+-----+
| theta  phi    chi   Rf/sigma |
+-----+-----+-----+-----+
|  1   44.85  75.39 156.15  12.13 |
|  2   96.89 174.67  93.49  12.03 |
|  3  120.19 144.37 113.66  11.61 |
|  4  135.60 -74.63 160.64  11.55 |
|  5   46.40  67.26 144.87  11.41 |
|  6  104.15 166.55  96.62  11.33 |
|  7  124.12 136.58 122.07  10.30 |
|  8  136.22 -82.74 172.28  10.13 |
|  9   45.60  71.53 150.64   9.88 |
| 10  100.81 170.52  94.76   9.49 |
| 11  135.90 -77.93 165.38   9.35 |
| 12  122.15 140.81 117.43   9.26 |
| 13  113.26 155.25 104.09   7.48 |
| 14   49.47  56.53 130.22   7.46 |
| 15   52.19  49.57 121.57   7.21 |
| 16  117.73 148.65 109.69   7.18 |
| 17   86.70 -174.47  92.96   7.06 |
| 18   43.73  86.85 172.40   6.94 |
| 19   89.14 -177.30  92.65   5.80 |
| 20   53.65 -165.60  29.92   4.31 |
| 21   53.65 -163.80  29.92   4.21 |
| 22   53.65 -167.40  29.92   4.20 |
| 23  110.61 -152.40 159.14   3.99 |
| 24  110.87 -152.10 160.20   3.95 |
| 25   53.65 -162.00  29.92   3.92 |
| 26  148.41 -144.30 158.96   3.92 |
| 27   14.16  41.70 163.12   3.90 |
| 28   94.42 117.30 157.66   3.88 |
| 29   94.12 117.00 157.44   3.83 |
| 30  141.04 -114.60 110.00   3.82 |
| 31  149.50 -143.40 160.29   3.81 |
| 32   78.28  81.00 174.80   3.81 |
| 33   94.13 108.30 118.50   3.80 |
+-----+-----+-----+-----+

```

(b)

```

Sol_best R1 R2  Rs Rself STF TF  PFmax  PFmin  TFCntr  Rfac  Scor
Sol_best  7  3   1  0  1  1  1.00  -13.73  0.000  0.531  0.215
Sol_best          Rot1->2          Dyad vector          dist d_ort          d_par
Sol_best          0.5  -73.0  15.6  -0.000 -0.000  0.402  110.7  1.0 110.7
Sol_best          Shift_1          Shift_2
Sol_best          0.671  0.685  0.199          0.671  0.685  0.601
Sol_best
Contrast = 4.542
Sol_          now number of found monomers: 4
Sol_          Final number of monomers: 4

```

Figure S3 Molecular Replacement Peaks. (a) MOLREP rotation function output showing peak heights. The first twelve peaks highlighted in yellow were the solution. (b) MOLREP translation output. The structure solution had a contrast value of 4.542 (light blue) that indicates that the model has a high probability of being correct. The search model was TcNDPK1 hexamer. Therefore, the 4 monomers (light blue) found by MOLREP translation function are actually 4 hexamers or 24 monomers that was the contents of the unit cell calculated from the Matthews coefficient.

Video S1 Live imaging of NDPK filaments incubated with different substrates. Images were captured using Olympus BX60 microscope with an Olympus XM10 camera. Videos were edited and accelerated 1000x with respect to the original playback speed. TcNDPK1 filaments were obtained in the absence of ATP stored at 4 °C, and incubated with AMP, ADP, ATP, dATP, GDP, GTP, dCTP, or dTTP (1 mM) and recorded.