Table S1: Hydrogen bonding and hydrophobic interactions between the different LdACT amino acid residues and DNA nucleotides.

| LdACT   | DNA     | Distance (Å) |
|---------|---------|--------------|
| (A) Hydrogen bonding                        |         |              |
| 38 ARG H21                                  | 46 CYT O5' | 2.3095       |
| 40 LYS HZ1                                  | 18 ADE O1P | 2.2023       |
| 41 ASN HD22                                 | 17 CYT O2 | 2.1272       |
| 43 GLN HE21                                 | 20 CYT O4' | 2.0254       |
| 43 GLN HE22                                 | 19 ADE N3 | 2.2320       |
| 43 GLN HE22                                 | 20 CYT O2' | 2.4343       |
| 48 SER HG                                   | 19 ADE O3' | 1.8594       |

| (B) Hydrophobic interactions                |         |              |
| 38 ARG CB                                   | 46 CYT C5' | 3.7733       |
| 38 ARG CB                                   | 46 CYT C4' | 3.6771       |
| 38 ARG CZ                                   | 46 CYT C5' | 3.8768       |
| 40 LYS CA                                   | 46 CYT C1' | 3.8917       |
| 42 MET CG                                   | 44 GUA C1' | 3.6864       |
| 42 MET CE                                   | 44 GUA C1' | 3.8583       |
| 43 GLN CB                                   | 19 ADE C4' | 3.5374       |
| 43 GLN CG                                   | 20 CYT C4' | 3.8562       |
| 45 MET CG                                   | 21 GUA C5' | 3.2745       |
| 48 SER CB                                   | 19 ADE C5' | 3.2931       |
| 48 SER CB                                   | 19 ADE C4' | 3.3288       |
Supporting Table S2

Energy statistics

| CNS energies (after water ref., kcal/mol) | LdACT:DNA |
|------------------------------------------|-----------|
| • $E_{\text{tot}}$                      | -17673.6  |
| • $E_{\text{bond}}$                     | 66.6      |
| • $E_{\text{angle}}$                     | 323.4     |
| • $E_{\text{improper}}$                  | 79.8      |
| • $E_{\text{dihed}}$                     | 2640.5    |
| • $E_{\text{vdw}}$                      | -2609.6   |
| • $E_{\text{electr}}$                   | -17574.5  |

r.m.s.d. from idealized geometry

|                                |           |
|--------------------------------|-----------|
| • r.m.s.d. $\text{bond}$(Å)  | 0.0031    |
| • r.m.s.d. $\text{angle}$(°) | 0.4831    |
| • r.m.s.d. $\text{improper}$(°) | 0.3986   |
| • r.m.s.d. $\text{dihed}$(°)  | 23.3148   |

PROCHECK analysis (full length amino acid 1-375)

|                                |           |
|--------------------------------|-----------|
| • Residues in most favoured regions (%) | 86.5      |
| • Residues in additional allowed regions (%) | 13.5      |
| • Residues in generously allowed regions (%) | 0.0       |
| • Residues in disallowed regions (%) | 0.0       |

Table S2: Thermodynamic analysis of LdACT DNA interactions.