# Acta Crystallographica Section D

**Volume 70 (2014)**

**Supporting information for article:**

## Structural analysis and insight into metal ion activation of the iron-dependent regulator from *Thermoplasma acidophilum*

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**Table S1** The absorbance measurements at 510 nm.

| Samples | Conc. (μ*M*) | Abs. (510 nm) | |
|---|---|---|---|
| | | No ascorbic acid | Ascorbic acid (100 m*M*) |
| *T. acidophilum* IdeR | 40 | 0.463 | 0.548 |
| $FeSO_4$ | 10 | 0.153 | - |
| | 20 | 0.290 | - |
| | 40 | 0.585 | - |
| | 80 | 1.177 | - |
| $FeCl_3$ | 10 | 0.028 | 0.104 |
| | 20 | 0.069 | 0.236 |
| | 40 | 0.185 | 0.480 |
| | 80 | 0.891 | 1.093 |

Data represent mean absorbance of three independent measurements.

The composition of Fe(II) was estimated to ~80% by calculation of (0.463/0.585)×100.

**Table S2** The distances between two residues in each dimer structure.

| | *T. acidophilum* IdeR (4O5V) | | Apo-DtxR (1BI2) | | Co(II)-IdeR (1FX7) | | Co(II)-IdeR-DNA (1U8R) | |
|---|---|---|---|---|---|---|---|---|
| | residues | distance (Å) | residues | distance (Å) | residues | distance (Å) | residues | distance (Å) |
| DNA recognition helix (α3) | | | | | | | | |
| Start | Lys40 | 37.4 | Ser37 | 35.0 | Ser37 | 31.4 | Ser37 | 33.7 |
| Center | Asp46 | 32.6 | Gln43 | 28.2 | Gln43 | 27.1 | Gln43 | 27.5 |
| End | Leu54 | 39.3 | Asp51 | 36.2 | Asp51 | 36.3 | Asp51 | 35.3 |
| Linker helix (α4) | | | | | | | | |
| Start | Pro69 | 49.9 | Pro66 | 47.5 | E66 | 49.7 | E66 | 49.6 |
| Kink | Leu79 | 27.7 | Met76 | 27.6 | Met76 | 27.8 | Met76 | 28.1 |
| End | Ile93 | 11.7 | Ile90 | 11.0 | Ile90 | 11.2 | Ile90 | 10.8 |