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Corrigendum

The structure of the TsaB/TsaD/TsaE complex reveals an unexpected mechanism for the bacterial t^{6}A tRNA-modification

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Subsequent to publication of this study, we obtained crystals that yielded slightly better diffraction data for the *Tm*TsaBDE complex (Table 1). These data resulted in improved electron density maps and allowed us to identify and correct a few errors in the previously deposited structure (originally deposited as PDB 6FPE). The latter (which is still available for download and comparison, at https://www.rcsb.org/structure/removed/6FPE) has been superceded by a new set of revised coordinates (PDB 6S84).

The most significant differences between the two coordinate sets consist of:

1. The C-terminus of one of the TsaB copies in the asymmetric unit: amino acids 194–205 that were missing in the 6FPE structure could be constructed into the density.
2. Modeling of a nucleotide bound at the active site of TsaD. We initially cautiously interpreted the residual electron density by glycerol and PEG moieties present in the crystal freezing liquor. The new maps clearly showed that a nucleotide was bound at this location (Figure 1). We could easily fit the density by AMPCPP, present as a ligand in the crystallization solution.

The new structure does not alter the primary conclusions of our manuscript:

- The C-terminal part of the active site of *Tm*TsaD remains well-structured and is still capable of binding a nucleotide in the context of the ternary *Tm*TsaBDE complex.
- The AMPCPP occupies exactly the same position as the carboxy-AMP compound present in the recent structure of *Tm*TsaBDE, reported by Swairjo *et al.* (1). We further confirm that in our structure the N-terminal part of the *Tm*TsaD active site remains partially disordered and that neither Zn nor Fe ions are bound. This contrasts with the structure reported by Swairjo *et al.*, which has an ordered metal binding site occupied by Zn. This latter structure was obtained in presence of ATP, and we suspect that the nature of the bound nucleotide (AMPCPP versus ATP) might play a role in the metal binding. The two structures of the TsaBDE complex (6N9A and 6S84) represent probably different snapshots along the catalytic pathway.

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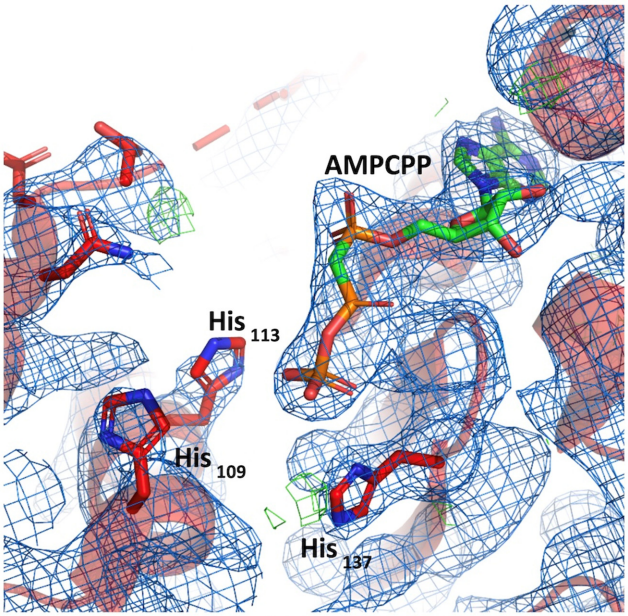

Figure 1. $2F_o$-F_c difference map (blue) of the AMPCPP surrounding at the active site of *Tm*TsaD. F_o-F_c map : positive and negative densities are represented as green and red grids respectively. The metal coordinating histidines 109 and 113 are also shown. They are partially disordered and not in a configuration compatible with metal binding.

Table 1. New (vs. original) data collection and refinement statistics

	PDB 6S84	**PDB 6FPE**
Wavelength (Å)	0.978570	0.9801
Resolution range (Å)	46.14–2.90 (3.00–2.90)	48.44–3.14 (3.33–3.14)
Space group	P 2_1 2_1 2_1	P 2_1 2_1 2_1
Unit cell a,b,c (Å)	a = 85.16, b = 108.21, c = 176.65	a = 84.31, b = 113.94, c = 177.62
Total reflections	324005	138146
Unique reflections	36849	30297
Completeness (%)	99.1 (94.8)	99.1 (95.2)
Mean I/sigma(I)	9.1 (0.87)	7.1 (1.03)
R-meas	0.23	0.19
CC1/2	99.7 (42.1)	99.2 (43.9)
R-work	0.209	0.23
R-free	0.282	0.29
Number of non-hydrogen atoms	10678	10418
RMSD bonds (Å)	0.003	0.011
RMSD angles (°)	1.011	1.258
Ramachandran favored (%)	94.77	95.3
Average B-factor ($Å^2$)	89.66	80.67

Statistics for the highest-resolution shell are shown in parentheses.

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