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CORRECTION

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Correction: Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase

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Correction for 'Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase' by Octav Caldararu *et al.*, *Chem. Sci.*, 2019, **10**, 576–586.

In the original article, two technical errors were made during the calculation of the nuclear scattering-length density maps for Fig. 2 and 3. As noted in the original article, joint refinement of the AA10 LPMO was conducted, even though the unit cells of the X-ray and the neutron crystals were slightly different (PDB IDs 5VG0 and 5VG1).[1] Both the traditional joint refinement and the quantum refinement were performed in the X-ray unit cell, but the nuclear density maps in Fig. 2 and 3 were calculated in the neutron unit cell. Furthermore, atom D1 was incorrectly considered as H when making Fig. 3B and D (all of the refinements correctly considered D1 as deuterium).

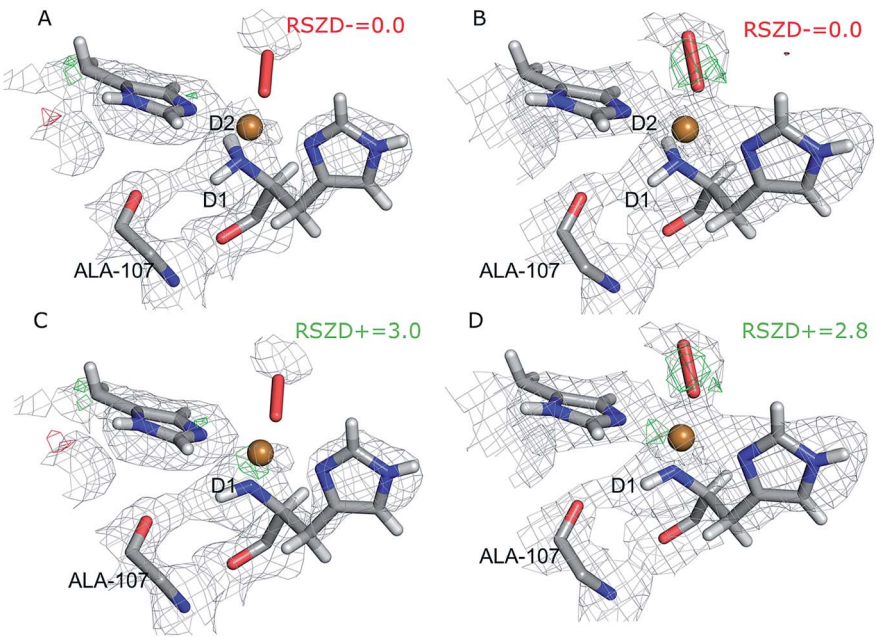

Fig. 2 Structure and nuclear density maps of the active site after joint refinement. The $m2F_o - DF_c$ maps are contoured at 1.0σ and the $mF_o - DF_c$ maps are contoured at +2.8σ (green) and −2.8σ (red). (A) – subunit A, ND_2; (B) – subunit B, ND_2; (C) – subunit A, ND^-, (D) – subunit B, ND^-. RSZD− values for the N-terminal atom are given for the ND_2 states to highlight if there are any extra atoms in the model. RSZD+ values for the N-terminal atom are given for the ND^- states to highlight if there are any missing atoms in the model.

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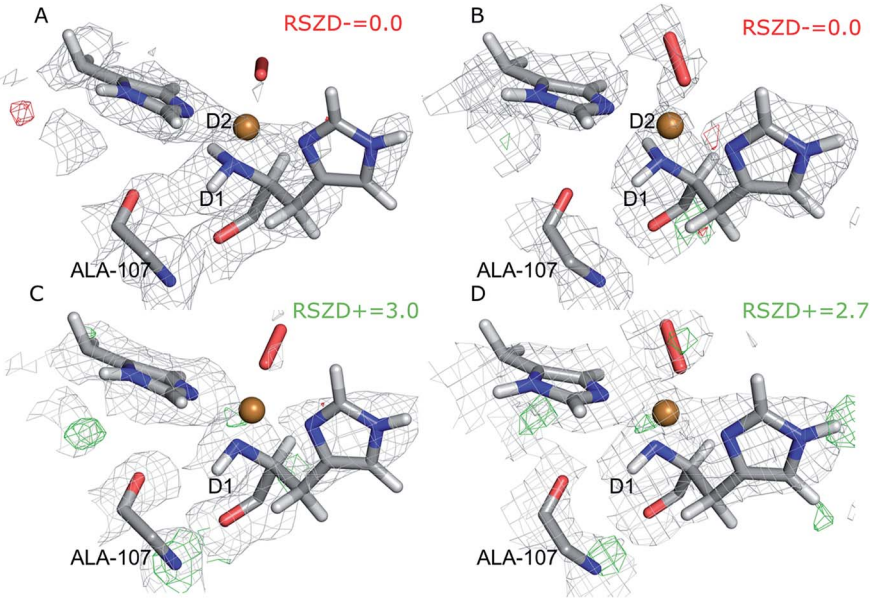

Fig. 3 Structure and nuclear density maps of the active site after quantum refinement. $m2F_o - DF_c$ maps are contoured at 1.0σ and $mF_o - DF_c$ maps are contoured at +2.8σ (green) and −2.8σ (red) (A) – subunit A, ND_2; (B) – subunit B, ND_2; (C) – subunit A, ND^-, (D) – subunit B, ND^-.

Corrected Fig. 2 and 3 are now reported as shown, with the nuclear density maps calculated in the X-ray unit cell and with the correct assignment of all of the deuterium atoms. The RSZD values for the N-terminus group have also been re-calculated.

The conclusions in the original article remain unaffected by these corrections. The structures with two deuterium atoms at the N-terminus show no negative difference density, neither in the traditional joint refinement nor in the quantum refinement. Removal of the D2 atom from the N-terminus gives rise to positive difference density in subunit B, although at a lower σ level than that reported initially (2.7–2.8σ compared to 3.2σ), but above the noise level of the nuclear density maps in that area (~2.3σ). While the maps without the D2 atom at the N-terminus show closer resemblance to those reported by Bacik *et al.*,[1] the structures with two deuterium atoms still fit better to the neutron data both in the traditional joint refinement and in the quantum refinement. Thus, the original conclusions about the protonation state of the N-terminus are unaffected by these corrections. The calculations suggest that the N-terminus is not deprotonated in the crystal structure.

The technical errors corrected above also do not affect the conclusions of the studies regarding the nature of the oxygen species and the mechanism of hydrogen peroxide formation by the AA10 LPMO presented in the original article.

Throughout the article, Glu-B65 was also consistently mislabeled as Glu-201.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

1 J. Bacik, S. Mekasha, Z. Forsberg, A. Y. Kovalevsky, G. Vaaje-Kolstad, V. G. H. Eijsink, J. C. Nix, L. Coates, M. J. Cuneo, J. Unkefer and J. C. Chen, *Biochemistry*, 2017, 8–11.