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Supporting information for article:

Serial femtosecond X-ray crystallography of an anaerobically formed catalytic intermediate of copper amine oxidase

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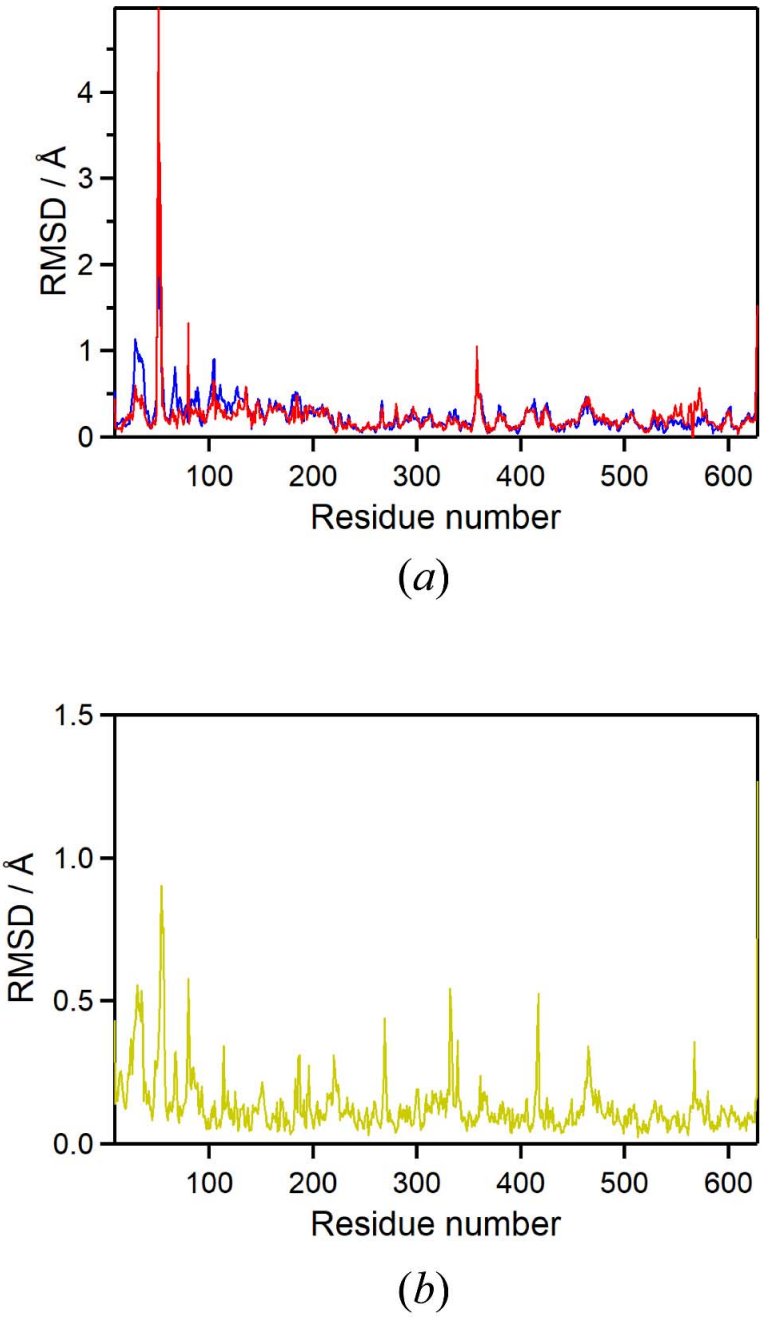

Figure S1 Comparison of average r.m.s. deviations (RMSD). (a) The RMSD values per residue of subunit A (blue) and subunit B (red) of the structure determined by the present SFX measurements were compared with those determined by the previous SFX using the grease matrix method (PDB entry 7f8k; Murakawa *et al.*, 2021) and plotted against the residue number. (b) The RMSD values per residue of subunit A of the structure determined in this study were compared with those determined by non-cryocooled X-ray crystallography using the HAG method (PDB entry 5zpn; Murakawa *et al.*, 2019) and plotted against the residue number.

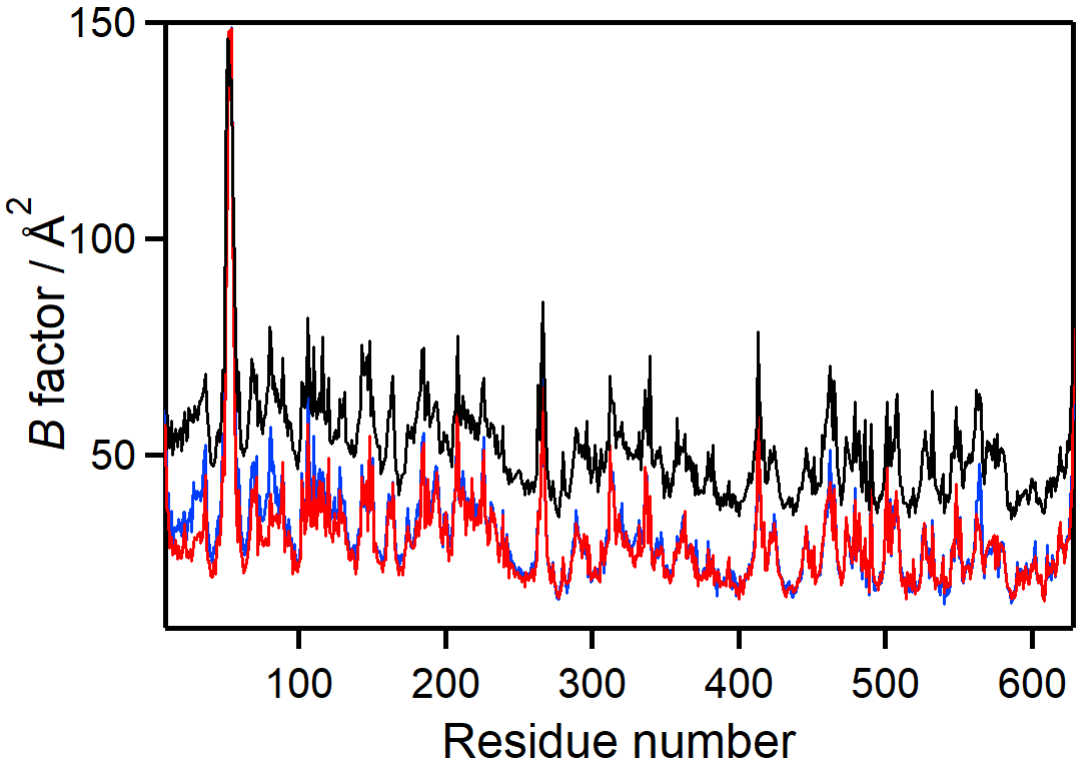

Figure S2 Distribution of atomic *B* factors. Average atomic *B* factors per residue in subunits A (blue) and B (red) of the structure determined by the present SFX measurements and that of the structure determined by the previous SFX using the grease matrix method (black, PDB entry 7f8k; Murakawa *et al.*, 2021) were plotted against the residue number.

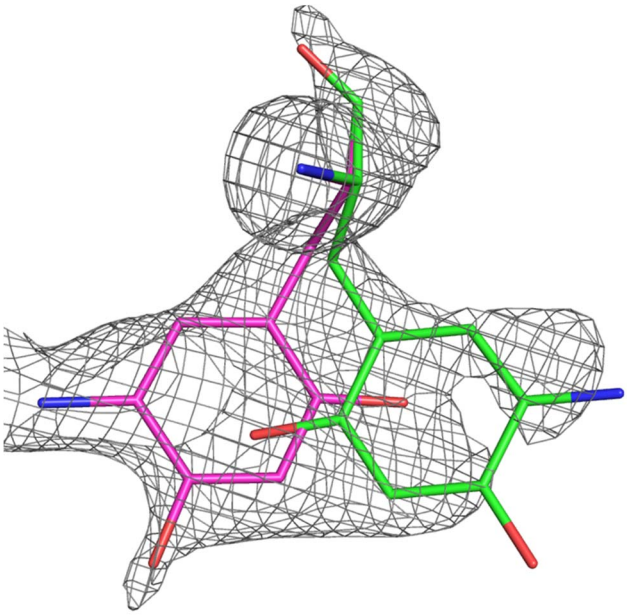

Figure S3 The refined structures and simulated annealing omit map of the TPQ cofactor. The assigned models of TPQ_{amr} (magenta) and TPQ_{sq} (green) are superimposed on the $F_o - F_c$ simulated annealing omit map for residue 382 that is contoured at 3.5 σ.