

Supplementary Information for

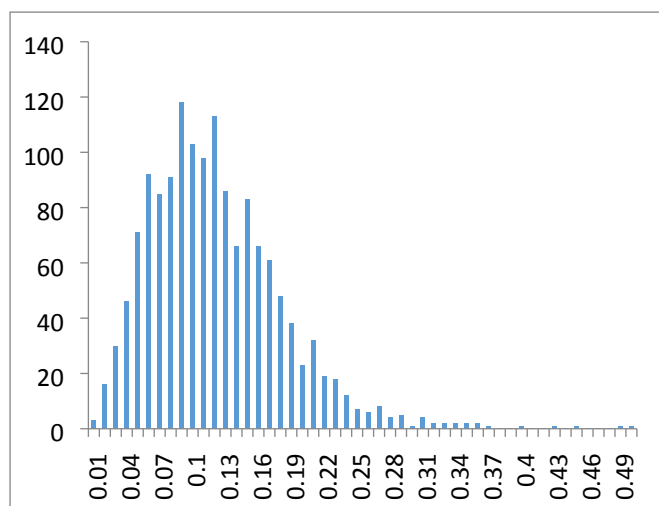
Structural perturbations of substrate binding and oxidation state changes in a lytic polysaccharide monooxygenase

Paul H Walton* and Gideon J Davies

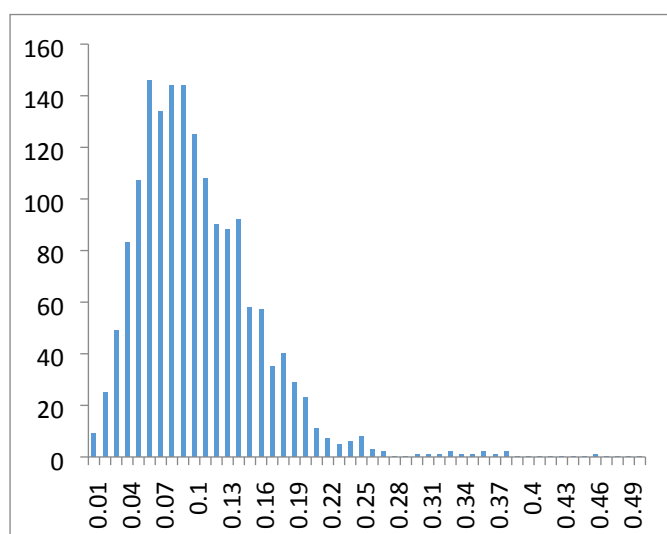
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Figure 1. Distributions of RMS values (all data). X-axis is pairwise RMS difference between equivalent atoms

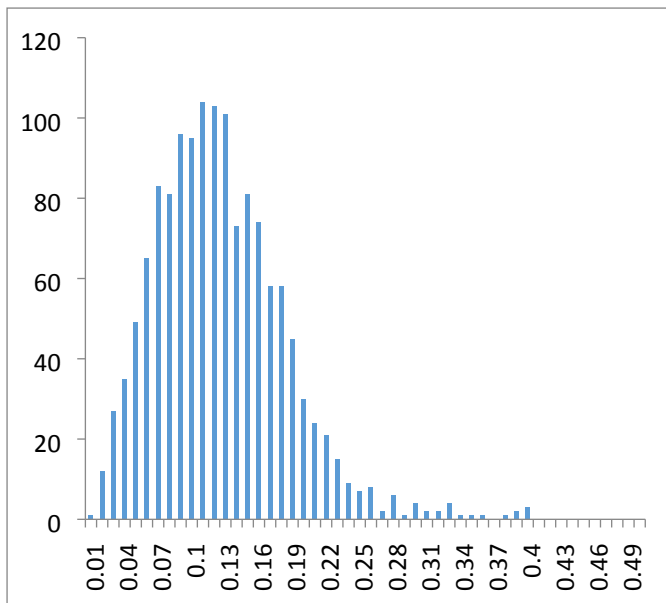
Cu(I) – Cu(II)



Cu(I) – Cu(I)G3



Cu(II) – Cu(II)G3



Cu(I)G3 – Cu(II)G3

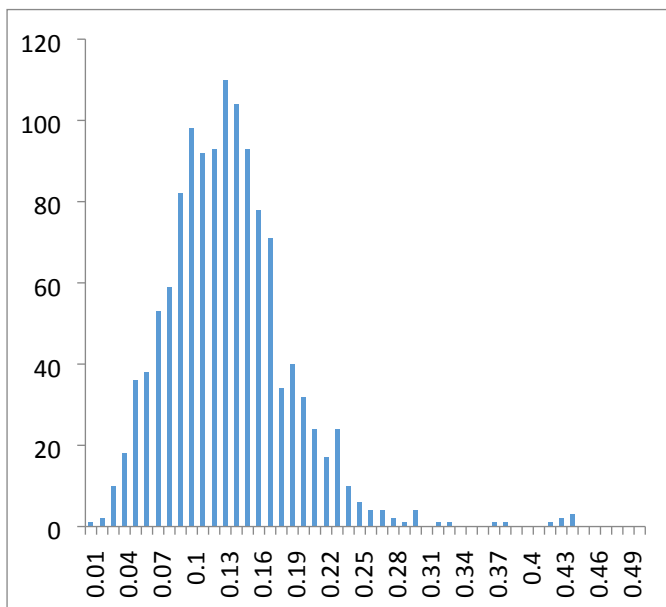
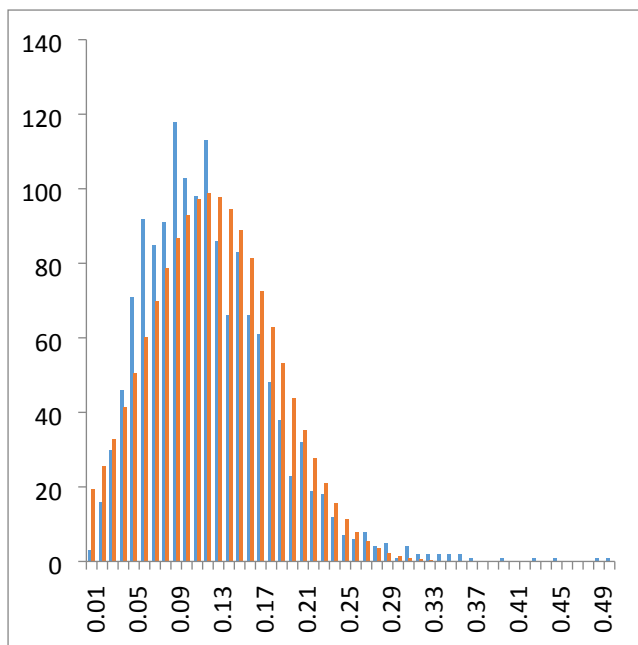
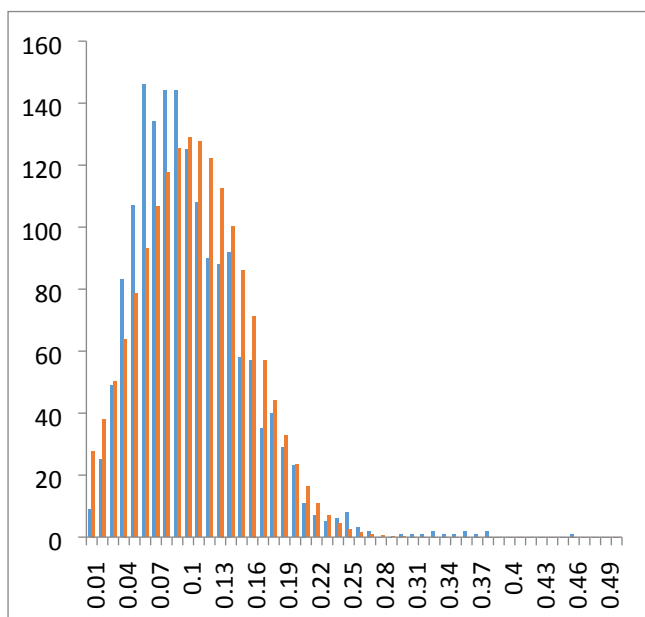


Figure 2. Comparisons of normal distribution histogram (orange columns) calculated from the use MoM parameters in the standard distribution equation for the pairwise comparisons of structures over the displacement parameter ranges as listed in Table 1 of the main text, and experimental data (blue columns). X-axis is pairwise RMS difference between equivalent atoms

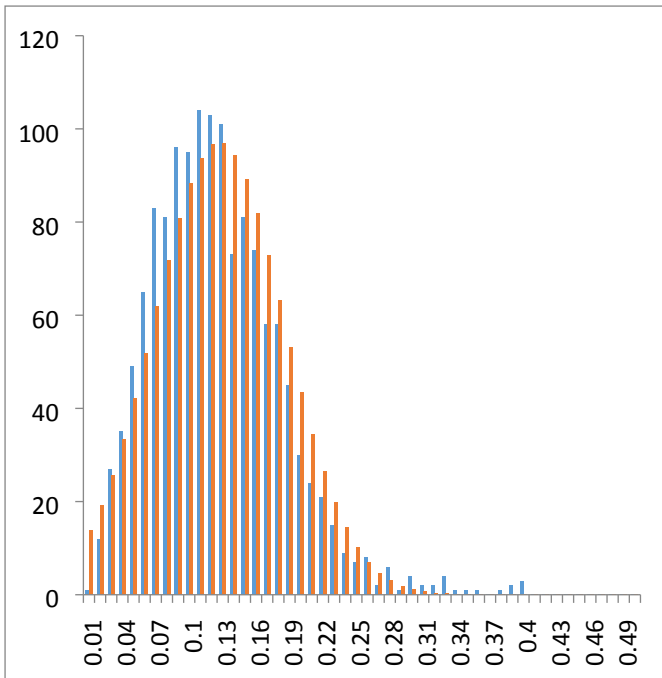
Cu(I) – Cu(II)



Cu(I) – Cu(I)G3



Cu(II) – Cu(II)G3



Cu(I)G3 – Cu(II)G3

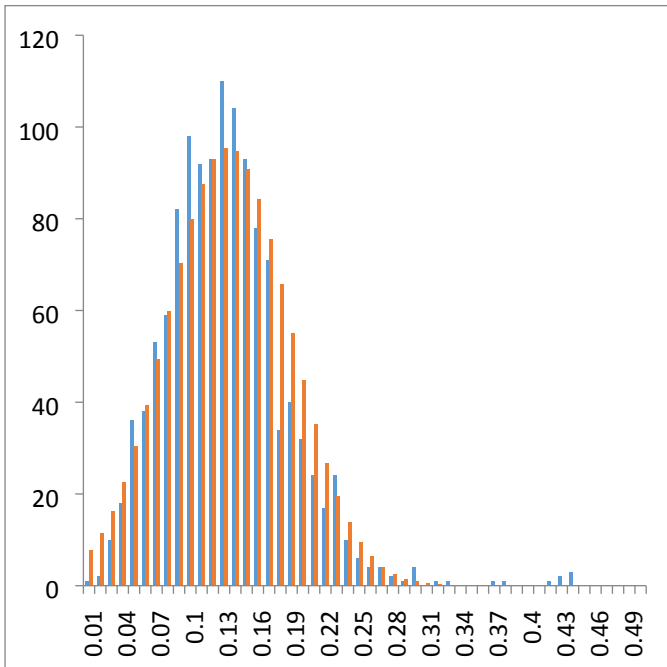
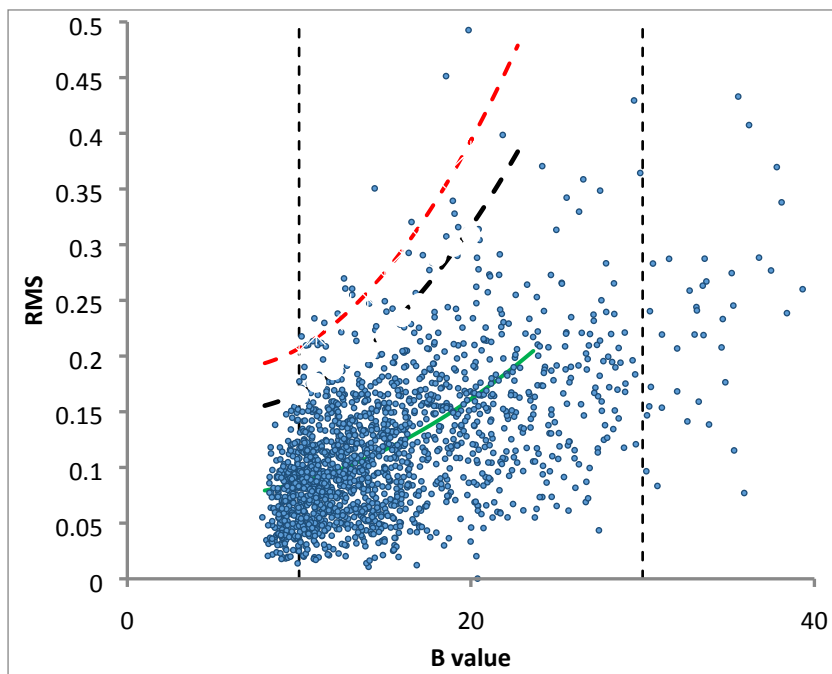
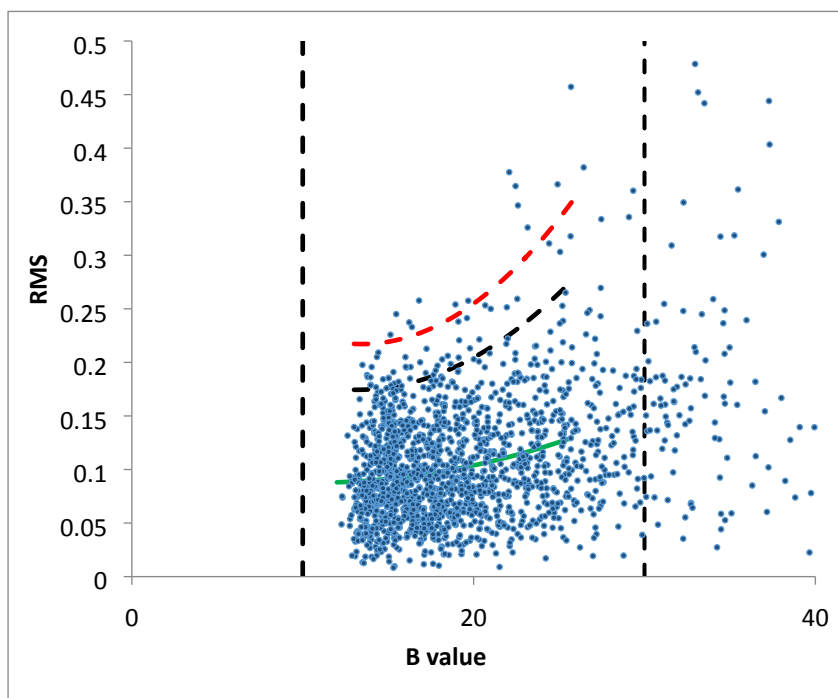


Figure 3. Plots of RMS differences between the atomic positions of pairwise atoms as a function of B-value, with estimators as a function of B value (green = mean, blue = $2 \times$ s.d., red = $3 \times$ s.d.). Vertical dashed lines represent the B-value ranges given in Table 1 of the main text.

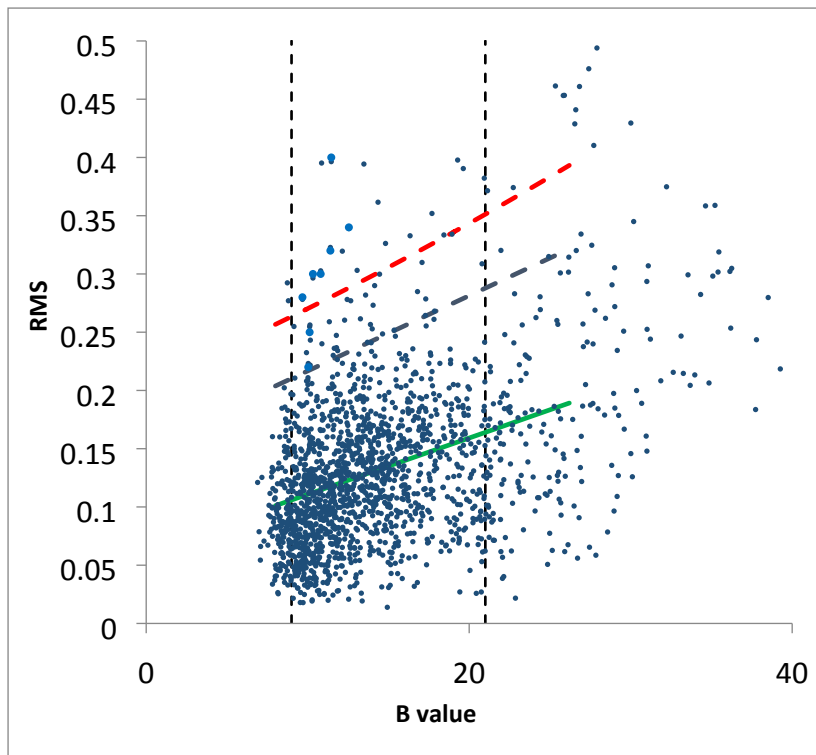
Cu(I) – Cu(II)



Cu(I) – Cu(I)G3



Cu(II) – Cu(II)G3



Cu(I)G3 – Cu(II)G3

