

Protonation State Determination In Proteins Using High Resolution X-ray Crystallography: Effects of Resolution and Completeness

S. J. Fisher, M. P. Blakeley, M. Cianci, S McSweeney, and J. R. Helliwell,

Supplementary Material

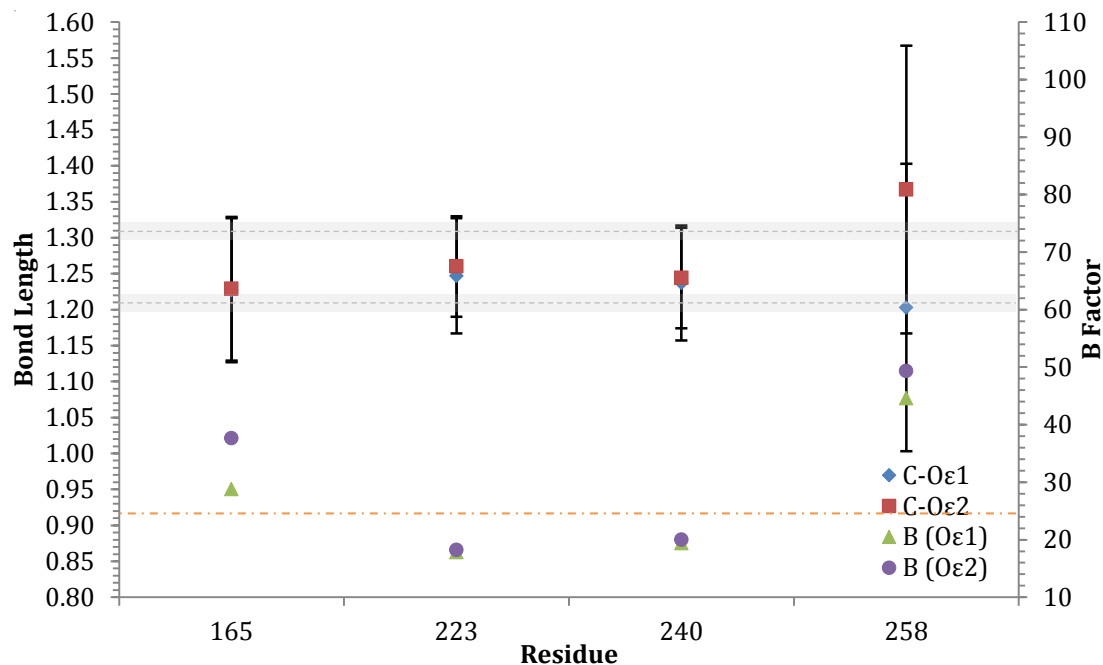


Figure S1: C-O Bond Lengths for Glu residues in cMyBP-C C1 domain at 1.3Å resolution. $B_{avg} = 24.4\text{\AA}^2$, $\sigma_{l(avg)} = 0.09\text{\AA}$. Adapted from (Fisher *et al.*, 2008).

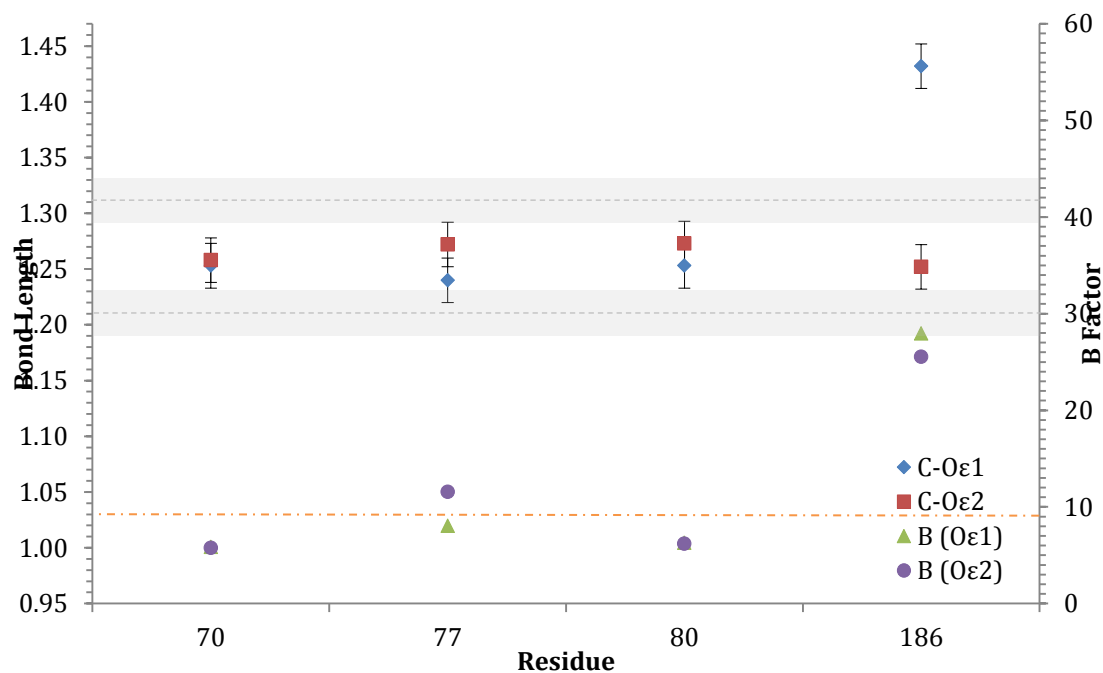


Figure S2: C-O bond lengths for Glu residues in bovine pancreatic trypsin. $B_{avg} = 10.0\text{\AA}^2$, $\sigma_{l(avg)} = 0.02\text{\AA}$

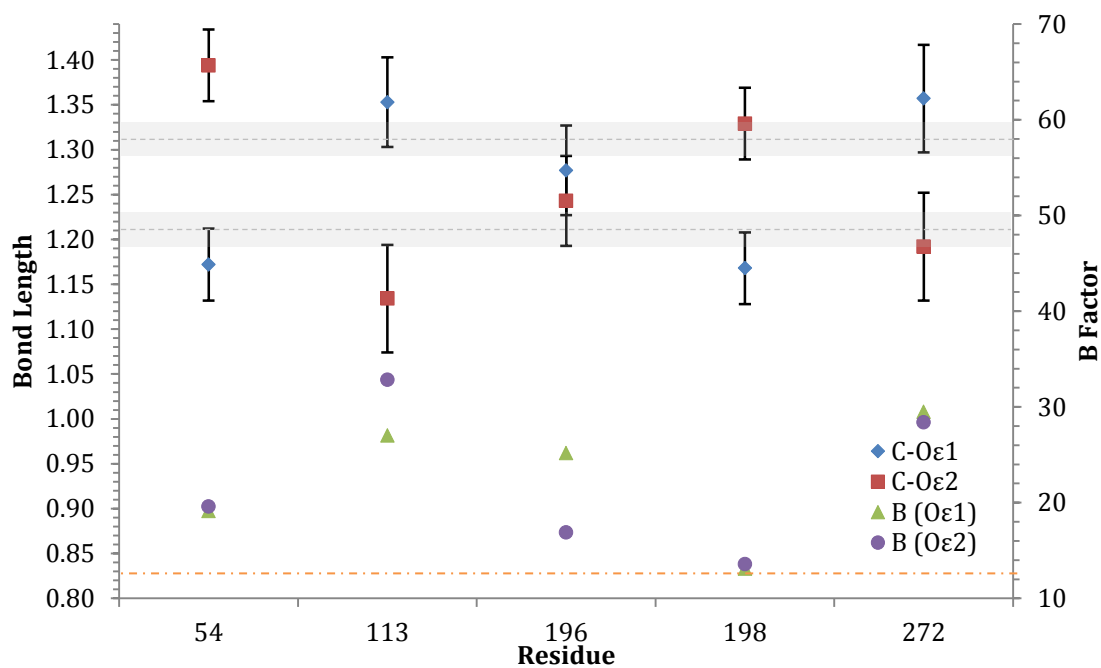


Figure S3: C-O bond lengths for Glu residues in subtilisin Carlsberg. $B_{\text{avg}} = 12.4 \text{ \AA}^2$, $\sigma_{l(\text{avg})} = 0.04 \text{ \AA}$

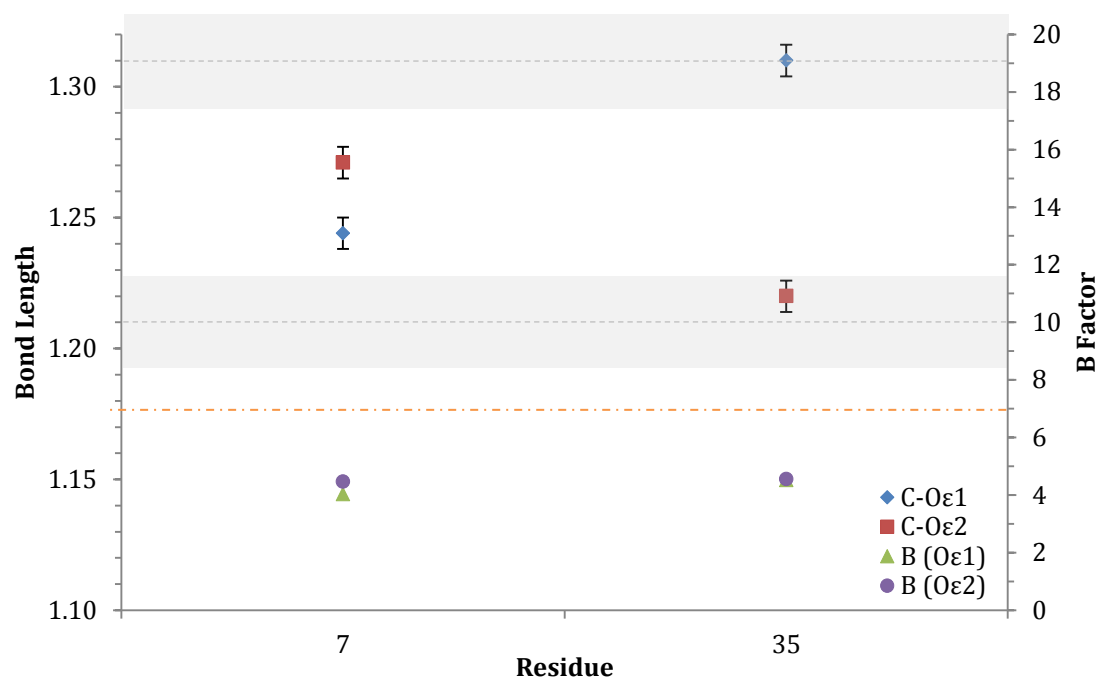


Figure S4: C-O bond lengths for Glu residues in Lysozyme. $B_{\text{avg}} = 7.1 \text{ \AA}^2$, $\sigma_{l(\text{avg})} = 0.008 \text{ \AA}$