

Microsymposium

MS100.O04

Validation of carbohydrate structures: not just nomenclature

J. Agirre¹, K. Cowtan¹

¹*Structural Biology Laboratory, Department of Chemistry, The University of York, England*

Despite the key implications carbohydrates have in a multitude of pathological processes, a large number of the sugar-containing structures deposited into the Protein Data Bank (PDB) show nomenclature errors [1] that persist even after the remediation of the PDB archive [2]. Here we present the results from a systematic study of the conformation and ring distortion of cyclic carbohydrate models for which structure factors have been deposited into the PDB. These models have also been scored using a real-space correlation coefficient calculated between model and experimental electron density. The results have enabled us to produce a database of well-refined carbohydrate structures for use in the framework of an automated sugar-detecting software, to be announced shortly.

[1] T. Lütteke, *Acta Cryst.*, 2009, D65, 156-168., [2] K. Henrick, Z. Feng, W.F. Bluhm et al., *Nucleic Acid Res.*, 36, D426-433.

Keywords: carbohydrate, validation, conformation