Validation of carbohydrate structures: not just nomenclature

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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.


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