Poster Presentation

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A knowledgebase of macromolecular non-covalent interactions including precision

J. Helliwell[1], M. Gurusaran[2], K. Sekar[3]

[1]*School of Chemistry, University of Manchester, UK,* [2]*Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore, India,* [3]*Supercomputer Education and Research Centre, Indian Institute of Science, Bangalore, India*

We have established a user knowledge base centred in Bangalore, but obviously accessible from anywhere in the world, for displaying ion pair distances for any protein deposited in the Protein Data Bank. We have published a description, its theoretical basis and examples of its use in IUCrJ [1]. The special characteristic is that the precisions on these distances is also displayed. These are based on the Diffraction Precision Index (DPI) approach [2] adapted to the pair of atoms involved in the non-covalent interaction and their specific B factors. Thus the display of the true precision can readily be seen by the user. We described other situations [1] where this approach could be used namely where restraints of a protein model refinement are not used such as metal ligand sites in proteins and protonation state determinations i.e. where a bond distance restraint is explicitly removed. We will report firstly on the ion pairs knowledgebase, as recently published, but with more examples from the user point of view. This will include a discussion of the range of precisions of the protein structures in the PDB as exemplified by using the DPI. Secondly, progress towards a knowledgebase, again including precision, for metal ligand interactions in the structures of metalloproteins and nucleic acids will be described.

[1] *M. Gurusaran, M. Shankar, R. Nagarajan, J. R. Helliwell and K. Sekar (2014). IUCrJ 1, 74-81.,* ***[2]*** *D. W. J. Cruickshank (1999). Acta. Cryst. D 55, 583–601.*

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