m34.p04

A Model for Coalescing Distributed Data Ontologies

Syd Hall[a], Nick Spadaccini[b], John Westbrook[c]

[a]School of Biomedical & Chemical Sciences, Univ. of Western Australia. [b]School of Computer Science & Software Engineering, Univ. of Western Australia, [c]Protein Data Bank, Rutgers Univ., New Jersey, USA. E-mail: syd@crystal.uwa.edu.au

Keywords: CIF, data ontologies, software design

COMCIFS, the IUCr Committee for the Maintenance of the CIF Standard, decided at the 2005 IUCr Congress in Florence to use the StarDDL [1] data ontology construction approach as a basis for coalescing existing collections of crystallographic definitions used to validate the CIF data items. Current CIF dictionaries are written using two languages commonly known as DDL1 and DDL2 [2] which are similar, but sufficiently different to pose obstacles for real definition portability and uniqueness, as well as for the efficient development of common CIF browsers and validators.
This paper will describe mechanisms for enabling the development of crystallographic data definitions as small modular ontologies that can be easily maintained and be coalesced, as needed, at instantiation time. This approach promotes uniqueness for defined definitions, thus avoiding the definition redundancy present across current dictionaries. The paper will also describe attributes that will facilitate the more routine use of ontologies for CIF data handling processes.

[1] Spadaccini, N., Hall, S.R., and Castleden, I.R. "Relational Expressions in STAR File Dictionaries" 2000 *J Chemical Information and Computer Science* 40, 1289-1301.
[2] International Tables for Crystallography (2005). Volume G, *Definition and exchange of crystallographic data*, edited by S.R. Hall & B. McMahon. Heidelberg: Springer.

m34.p05

High resolution crystallography and electrostatic interaction energy computation

A. Lagoutte, B. Guillot, V. Pichon-Pesme, S. Pillet, C. Jelsch, C. Lecomte

LCM3B, UHP Nancy1, FranceE-mail: angelique.lagoutte@lcm3b.uhp-nancy.fr

Keywords: high-resolution X-ray crystallography, electrostatic interaction energy, databases

The PDB records show the number of (ultra-)high resolution biological macromolecules X-ray structures increasing quickly. Feasibility of multipolar refinement of such structures has been proved [1], assuming subatomic resolution and sufficiently low thermal motion. The Hansen & Coppens atom model gives an analytical representation of the charge density. It enables the experimental estimation of charge transfer, electrostatic potential and interaction energy. As the electrostatic properties are of major importance in numerous biological processes (catalysis, molecular recognition, ligand binding), computing electrostatic interaction energy could help in the analysis of the structure-function relationship, and provide information related to biological macromolecules activity. We will present the advancement of the crystallographic software VMoPro and a method to calculate protein-ligand electrostatic interaction energy. This program allows us electrostatic potential calculation, charge density topology, static electron density and to visualize it in 3D-maps. The energy computation, developed in our software, is an elaborated numerical integration of the product of a (ligand) charge density and a (protein) electrostatic potential, both obtained from the VMoPro software [2]. The protein electron density parameters will be either refined or transferred from our charge density database [3] in case of atomic resolution. To obtain the total electrostatic energy, the van der Waals energetic contribution, and the penetration electrostatic component [4a, 4b] shall be added. We will present our results on small molecules, urea and on two DNA bases: anhydrous cytosine and ribonucleotide thymidine. These latter two crystal structures were collected at ultra-high resolution at the ESRF synchrotron, on the Swiss-Norwegian Beam-Line [5]. We carried out a multipolar refinement to extend our experimental database modelling DNA. The charge density refinement will be discussed.

[1] Jelsch, C; Teeter, M. M.; Lamzin, V.; Pichon-Pesme, V.; Blessing, R. H.; Lecomte, C.; *PNAS*, 2000, 97, 3171.
[2] Jelsch C., Guillot B., Lagoutte A., Lecomte C., *J. Appl. Cryst.* A, 2005, 38, 38.
[3] Pichon-Pesme V., Jelsch C., Guillot B., Lecomte C., *Acta Cryst.*, 2004, A60, 204. [4a] Spackman, M. A.*; J. Chem. Phys.*, 1986, 85, 6579. [4b] Spackman, M. A.; *J. Chem. Phys.*, 1986, 85, 6587.
[5] http://www.esrf.fr/exp_facilities/BM1A/index.htm