m34.p10

An Analysis of Ligand Structures in the Protein Data Bank

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Keywords: ligand, conformation, internal strain

There have been a number of ligand structures deposited in the Protein Data Bank (PDB) in questionable conformations. Although the availability of structure factors for most of the PDB is sadly lacking, public deposition of structure factors for some models provides an opportunity for further analysis. We have re-solved a number of ligand structures using a protocol that accounts for both strain energy and experimental data in a rigorous fashion. The strain energy and conformational differences, and agreement with experiment of the alternate solutions will be presented. In addition, examples of improbable structural motifs will be provided.

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The CCP14: freely available crystallographic software for academia (collaborative computational project number 14)

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Because of the large scope of applications for single crystal and powder diffraction software; a way to think about how the CCP14 website is structured is to consider it as a large ***"Jeweller's Shop"***. However, unlike a Jeweller's Shop all the material is ***freely available*** for academic and student use. You may or may not know what you are after exactly. Or only have a general idea of what your needs are. Given the wide scope of single crystal and powder diffraction; there are many options and possible pathways. The optimum pathway on choosing the most appropriate software to use could involve minor nuances in your research requirements. The CCP14 project encourages a genetic diversity of software and methods so you may find a variety of software that has similar functionality; but may have specialist features beneficial in certain circumstances. One recommendation is to try a variety of relevant programs to help generate your personal software toolset. Doing this as part of developing the computational and analytical resources of your laboratory can be very beneficial compared to just using the first software program that comes to hand. Many software programs with similar functionality can be complementary and enable cross validation of results. The Graphical Site Map may help you find what you are after. It lists the main areas plus the most popular resources. The Free Text Site Search: is now fast and good for data-mining of complex queries. It has ″Relevancy Scoring″ plus if you know what you are after but cannot be bother browsing the menu systems - just enter it here. (e.g., WinGX)

Some Starting Points
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Text Site Search: The latest SWISHE and Google/Yahoo search engines should be lightning fast to run.
Web based Tutorials: See before you try
Methods, Problems and Solutions: Pages guided by queries people have asked in the past
Mirrored Software and Websites: Saving time by using a CCP14 based mirror
Developer Resources: Freely Available Source Code, Compilers and related material

[1] *http://www.ccp14.ac.uk/*