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Ligand's Den: PURY Based Hetero Molecules' Geometry Validation Server. Miha Andrejašič[a], Dušan Turk[a]. [a]*Department of Biochemistry, Molecular and Structural Biology, Jožef Stefan Institute, Ljubljana, Slovenia.*
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Whereas interactive web based tools for validation of structures of biological polymers are regularly used during macromolecular structure refinement and deposition process, tools for validations of hetero compounds have not yet been made available. As a result, the structures of small molecules found in complexes with biomacromolecules are commonly less reliable than those of the surrounding amino and nucleic acids. The increasing number of complexes of hetero compounds however requires fast of this problem. Therefore a web-based tool for interactive validation of small molecule ligands in complexes with macromolecular structures has been made available to public use (for holders of CSD license). The validation server is based PURY database of geometric restraints of hetero molecules (Andrejasic et al., 2008) which is derived from crystal structures of small molecules deposited CSDB by statistical analysis. Bond length and bonding angles of deposited molecules are compared with their corresponding PURY targets. Validation report is based on deviation from the target value measured in standard deviations of each particular term. The under laying software has been used to validate geometry of hetero compounds already deposited in PDB. This validation report will be presented; most common problems together with most erroneous cases will be exposed.

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Keywords: macromolecular X-ray crystallography; structural analysis software; Cambridge structural database

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X-Ray Tomography on MX Samples. Sandor Brockhauser[a], A. A. McCarthy[a], M. Di Michiel[b], J. E. McGeehan[a,c], R. B. G. Ravelli[a,d]. [a]*EMBL-Grenoble, France.* [b]*ESRF, France.* [c]*University of Portsmouth, UK.* [d]*Leiden University Medical Center, The Netherlands.*
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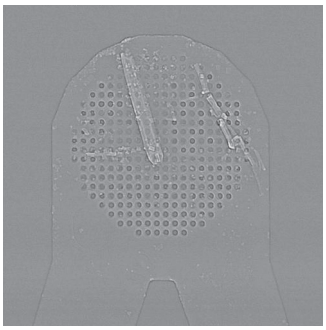
The anomalous scattering properties of innate sulphur can be used to solve the phase problem in macromolecular crystallography (MX) via the SAD method. However, this method, which is used at longer X-ray wavelengths (1.5 – 2.5 Å), is still not a routine tool in MX. One of the difficulties associated with the longer wavelengths, is the increased absorption from both air and sample. So far, only empirical absorption algorithms exist, because of the difficulties of routinely and precisely measuring the shape of the absorbing objects. In this report [1], we present the use of X-ray microtomography to reconstruct the 3D shape of crystal, surrounding solvent and sample holder. The setup can be integrated within a general MX environment. The dose needed for the tomographic measurements could be low enough to allow the technique to be used for crystal integrity characterization and alignment.



[1] S. Brockhauser, M. Di Michiel, J.E. McGeehan, A.A. McCarthy and R.B.G. Ravelli, **2008**. *J. Appl. Cryst.* 41, 1057-1066.

Keywords: X-ray tomography; crystal shape; protein crystallography