Poster Presentation

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How databases can help set standards from validation to publication

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Databases can play a key role in structure validation and can play their part in setting standards from validation to publication.

The Cambridge Structural Database (CSD) currently contains over 875,000 organic and metal-organic crystal structures. The wealth of information in such a database can help increase the integrity and validity of new structures. The knowledge derived from the entries in the CSD is already being used by crystallographers worldwide in small molecule and protein structure validation.

One key area where databases can help the crystallographic community set standards is through interactive deposition processes. During a deposition process the format of the data can be set to adhere to community standards and the inclusion of associated data such as structure factors, can be mandated or encouraged. Deposition processes could also include checks and measures to help crystallographers identify and fix issues prior to publication and could help the community set new standards.

This presentation will focus on what the CSD and other crystallographic databases currently do in terms of setting standards and will explore the role databases could play in the future to help the crystallographic community to set new standards from structure validation to publication.

Keywords: Databases, standards, validation