

# The Use of Stereo Descriptors in the Context of a Structure Validation Workflow

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The proper interpretation of a chemical structure drawing within a chemical information system is essential for storage and retrieval as well as for the analysis of chemical structures. A Structure Validation workflow will go through several stages of structure examination in order to verify consistency with proprietary drawing rules and to identify stereochemical features. This presentation describes these stages with particular focus on the stereochemical analysis. The latter relies on a robust, accurate, and high performing CIP calculator, which was developed in a joint collaboration of scientists and software engineers. The range of stereochemical descriptors provided by this calculator includes regular Cahn-Ingold-Prelog stereodescriptors as well as descriptors for identifying stereocentres which are not explicitly specified (hidden) in a given structure drawing or which are incorrectly drawn.