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Quantum crystallographic evaluation of the YLID crystal structure; reconsidering data quality

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YLID crystals have been used as test crystals for X-ray diffractometers. But, no charge density evaluation has been performed for this crystal. It is certainly more meaningful if we compare, e.g., hydrogen anisotropic displacement parameters and the residual density distribution to evaluate our diffractometer. So, for data quality evaluation of a diffractometer, quantum crystallographic procedures are helpful.

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