IDEAL - Invariom Derived Electron AnaLysis for APEX3

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With the introduction of large shutterless detectors, data quality to high resolution has dramatically improved over the last few years. Data to 0.5 Å and beyond can be collected with only one detector setting, with short exposure times, and short overall experiment times. Traditionally structures are refined using an Independent Atom Model (IAM), although good data beyond the traditional 0.83 Å reveals additional electron density that cannot be modeled appropriately. Often practitioners choose to cut data to preserve a low structure reliability criteria R1, sacrificing additional information and overall structure quality.

IDEAL lets you have the cake and eat it too! IDEAL uses a database of bond-oriented deformation density parameters derived from the invariom[1] database of *ab initio* calculations of model compounds. IDEAL generates BEDE (Bond Electron Density) and LONE (Lone Pair Electron density) for refinement with an extended version of XL. XL uses IAM scattering factors and in addition, models scattering contributions of bonds and lone pairs.

IDEAL delivers structures with increased model accuracy and provides access to more detailed model properties. IDEAL is easy to use and seamlessly integrated with APEX3 and SHELXle.

[1]The generalized invariom database (GID)
B. Dittrich, C. B. Hübschle, K. Pröpper, F. Dietrich, T. Stolper and J. J. Holstein Acta Crystallogr B, Struct Sci Cryst Eng Mater. 2013 Apr; 69(Pt 2):91-104