What To Do When *H*, *K* And *L* Do Not Describe All the Reflections in The Diffraction Pattern?

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Here I will present a recently determined crystal structure of ipragliflozin L-proline, a pharmaceutical drug used for the treatment of type 2 diabetes. Due to the small crystal size, MicroED was used to determine this structure. Initial phasing was carried out in the orthorhombic space group $P2_12_12_1$, but refinement in this space group proved to be challenging. Subsequent reduction in symmetry to $P2_1$ produced a structure that could be refined, and this structure was published earlier this year (Shah, *et. al.* 2023). Further inspection of the raw diffraction data revealed unindexed spots indicative of overlooked incommensurate modulation. I will discuss the implications of this modulation and possibly some further attempts to better handle these data.

Structure in the CCDC: FEXJIF (2174023) Raw Data: DOI 10.5281/zenodo.7308613 Shah HS, Yuan J, Xie T, Yang Z, Chang C, Greenwell C, Zeng Q, Sun G, Read BN, Wilson TS, Valle HU, Kuang S, Wang J, Sekharan S, Bruhn JF. Absolute Configuration Determination of Chiral API Molecules by MicroED Analysis of Cocrystal Powders Formed Based on Cocrystal Propensity Prediction Calculations. Chemistry. 2023 Mar 7;29(14):e202203970. doi: 10.1002/chem.202203970. Epub 2023 Feb 6. PMID: 36744589.