

Protein crystals are ~50% “solvent”. What is “solvent”?

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Even though protein crystals are roughly 50% solvent by volume, the composition and structure of that solvent is not readily accessible in crystallography. These are important in both quantitatively determining and assessing electron density maps [1], and in simulations of protein and solvent dynamics in crystals [2]. The usual initial assumption, that the internal solvent has the same composition and density as the solvent the crystals are soaked or grown in, fails to account for the effects of solvent nanoconfinement and interactions with the protein [3].

We have attempted to measure the composition and density of solvent within protein crystals using robust methods that can be broadly applied. We will describe our methods and results for two different protein crystal systems and compare them with results of crystallographic analyses on the same crystal systems.

References

[1] Lang, P. T. *Et al.* (2014). *PNAS*, **111**, 237-242

[2] Janowski, P. A. *et al.* (2016). *Protein Sci.*, **25**, 87-102.

[3] Moreau, D. W. *et al.* (2019). *IUCrJ*, **6**, 3.