Invited Lecture

Automation in small-molecule crystallography: Capabilities and challenges

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There is so much automation all around us, and our daily lives rely heavily on it, but we rarely stop and think about it (mostly only when it goes wrong!).

When driving a car, we take for granted that it 'just works'. We concentrate on navigating the vehicle from A to B safely. The car 'just working' results from many decades of advances in engineering and a great deal of automation.

The same is true for crystal structure analysis: We assume that crystallographic software 'just works' and we have become utterly dependent on it. Modern crystallographic software is based on a high degree of automation, even though we don't usually think about it this way. On the contrary, many crystallographers see increasingly automated software as a threat for various reasons.

However, it's important to note that automation in crystallography isn't about surrendering control. It's about enhancing our capabilities, streamlining processes, and, ultimately, advancing our understanding of crystal structures.

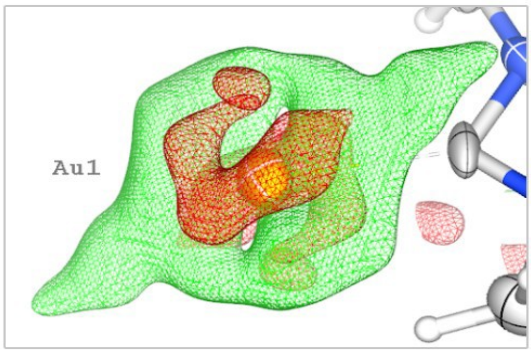
Many—if not most—crystal structures are determined and published by interested chemists rather than professional crystallographers. Anyone interested in atoms and molecules can perform decent structural analyses with modern instrumentation and software (and a little online help).

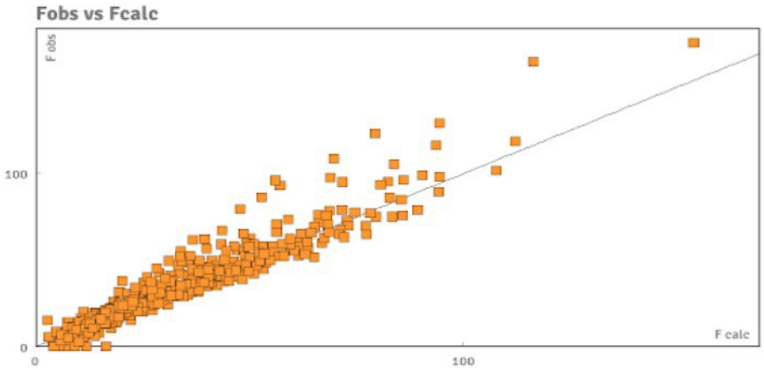
In this contribution, I will highlight some lesser-known areas where automation plays a role in crystallographic software and show how this helps and rarely hinders.

Crystallography (and chemistry!) is extremely lucky to have a well-functioning 'watchdog': The IUCr issues detailed guidelines, and the CheckCif concept is second to none in science. Yet, problematic structures can and do surface in the literature.

Crystallographic teaching is—if it happens at all—too often geared towards the car's inner workings and not towards driving it. While we rely on mechanics and engineers (and we better ensure that these will always exist and continue developing ever-better software and techniques!), ensuring that those using crystallography as a tool can do so safely and with scientific integrity is of much higher importance in general crystallographic education.

The central part of this contribution will consist of an instructive and entertaining tour-de-force through the most frequently encountered mistakes in small-molecule crystallography. I will highlight their source and how anyone can catch these errors before submitting a structure to a journal for publication.





Almost all real crystallographic issues with a structure can be readily diagnosed by examining the residual density maps in conjunction with a combination of relevant statistical graphs. Finding a reason for an observed issue may not always be easy, but it is always possible to see that a problem exists.

With experience and education, we will all become better at identifying and diagnosing problems. However, there will always be times when this is very difficult, and taking the car to the garage might be necessary. Make sure it's a friendly garage that will let you watch and learn!