

George Sheldrick's SHELX: success for all

I. Usón^{1,2}

¹ *Instituto de Biología Molecular de Barcelona (IBMB-CSIC), Barcelona Science Park, Baldiri Reixach 15, Barcelona, 08028, Spain,* ² *ICREA, Institució Catalana de Recerca i Estudis Avançats, Passeig Lluís Companys 23, 08003 Barcelona, Spain*

uson@ibmb.csic.es

Success for all was the motto of Huddersfield New College, George's school in the town where he was born. George not only learned chess and German there, he graduated in a much larger number of courses than was needed, or indeed usual, obtaining nine O-levels, six A-levels and two S-levels. At A-level, he achieved a distinction (the highest grade) in physics, mathematics and chemistry. George was awarded a Major Scholarship to study at Jesus College, Cambridge; at the time he was the only student in Jesus College to come from a non-private school. The school seems to have had a lasting influence, in line with the importance of education. If the motto encapsulates a school's ethos and guiding principle, George took it with him throughout his career.

SHELX transformed crystallography, empowering researchers across chemistry, mineralogy and biology, in words of crystallographers in the 70s and 80s, *SHELX* democratized crystallography. In one of the most cited papers ever (Sheldrick, 2008), George describes the birth of the *SHELX* programs [1] and their robust design with zero dependencies and upwards compatibility. The present talk will outline George Sheldrick's contributions along the development of the *SHELX* suite and illustrate their impact. We will be looking into the early *SHELX76* and the achievements it mediated by contriving original solutions to make the most of the limited computing resources. The extension of phasing methods and the quest for structure solution exploiting direct methods, phase annealing and the Patterson function used as bias in *SHELXS*. Extension to the solution of macromolecules with dual-space recycling in *SHELXD* for *ab initio* or substructure phasing and high throughput experimental phasing with *SHELXC*/*SHELXD*/*SHELXE* and its *sphere of influence* [2] or to their refinement in *SHELXL*[3]. George's contribution to data processing in the programs written for Bruker hardware like *SADABS* could not be absent from this sketch. *SHELXT* [4], the last member of the *SHELX* suite integrates structure solution with space group determination and element assignment, and was written in one sweep as George knew exactly what he wanted to program and, once written, it all worked according to plan and like his other programs has contributed to the success of many scientists.

[1] Sheldrick, G.M. (2008). *Acta Cryst.* **A64**, 112–122.

[2] Sheldrick, G. M. (2002). *Z. Kristallogr.* **217**, 644–650.

[3] Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.

[4] Sheldrick, G. M. (2015). *Acta Cryst.* **A71**, 3–8.

Too many contributions to name individually are acknowledged for providing feedback, setting facts right and expressing thoughts about George's life, work and impact.