Forensic Crystallography – or how to improve your stubborn refinement

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You have good data, an apparently good model and no startling validation alerts, yet your R-factor remains stubbornly high. What can one do? It helps to develop one's own mental toolbox for detecting as yet unresolved aspects of a structure refinement and simply being observant and correctly interpreting what the structure is trying to tell you. The discussion will include some ideas for recognising or discovering subtle indicators of when further improvements might be made to the model or data processing. Our eyes are great at seeing things like strange-looking atomic displacement ellipsoids in a model – if it looks strange, it probably is. Delving into output files, such as the SHELXL *.lst file, can be revealing, yet with such nice software tools and GUIs these days, one quickly forgets the importance of glancing at such output files at least once per structure determination. Examples will include detecting more than one chemical compound on the same crystallographic site, ensuring H-atoms are appropriately positioned, refinement finalisation with inversion twins, and ensuring the final model is chemically logical.