



## The Definitive Hitchhiker's Guide to Pathological Macromolecular Crystals Editorial for Crystallography Reviews, Issue 1 of 2020

Petra Bombicz

To cite this article: Petra Bombicz (2020) The Definitive Hitchhiker's Guide to Pathological Macromolecular Crystals Editorial for Crystallography Reviews, Issue 1 of 2020 , Crystallography Reviews, 26:1, 1-2, DOI: [10.1080/0889311X.2020.1714861](https://doi.org/10.1080/0889311X.2020.1714861)

To link to this article: <https://doi.org/10.1080/0889311X.2020.1714861>



Published online: 28 Jan 2020.



Submit your article to this journal [↗](#)



Article views: 53



View related articles [↗](#)



View Crossmark data [↗](#)



## The Definitive Hitchhiker's Guide to Pathological Macromolecular Crystals

### Editorial for Crystallography Reviews, Issue 1 of 2020

As the authors say, they give a 'The Definitive Hitchhiker's Guide to Pathological Macromolecular Crystals' in their tutorial review article 'Characterizing pathological imperfections in macromolecular crystals: lattice disorders and modulations' by Jeffrey J. Lovelace and Gloria E. O. Borgstahl from The Eppley Institute for Research in Cancer and Allied Diseases, University of Nebraska Medical Center, Omaha, USA. Four main categories of pathological crystals are described from the easiest to the most difficult: rotational order/disorder (ROD), layer translocation defect (LTD), translational non-crystallographic symmetry (tNCS) and modulation. The paper provides an easy to follow experimental pathway to solve each malady, the descriptions of crystal issues are given, the symptoms and ways of solution are detailed.

The review article 'Introduction to crystallographic refinement of macromolecular atomic models' by Alexandre G. Urzhumtsev from the IGBMC, CNRS-INSERM Illkirch and Université de Lorraine, Nancy, France and Vladimir Y. Lunin from Keldysh Institute of Applied Mathematics of Russian Academy of Sciences, Moscow, Russia [1] is now accomplished with an addendum by the authors. The review section '5.8.2 Subatomic resolution' is completed with some historical details, especially with a reference of a forgotten article by Rosalind Franklin in Nature [2]. Franklin showed in 1950 the impact of bond electrons on structure factors, moreover she modelled their contribution as that from point scatterers at the middle of bonds. This was the first attempt on modelling of deformation density.

A Statement by Dietmar Stalke, Regine Herbst-Irmer and their co-workers from the Institute for Inorganic Chemistry, University Göttingen, Germany is issued on the review 'Metrics for crystallographic diffraction- and fit-data: a review of existing ones and the need for new ones' from Julian Henn [3] as he refers two of their examples as case studies. The overall aim is to improve X-ray structure analyses, addressing issues with  $\sigma(I_o)$ s, as well as to avoid overfitting in charge density models. The community of Crystallographers is aware of the need for improvement in hardware and software and the upcoming developments towards data quality need to be discussed.

The book 'Data analytics for protein crystallization' edited by Marc L. Pusey and Ramazan Savaş Aygün in 2017 is part of the Computational Biology series of Springer International Publishing AG. It was reviewed by Ivana Kuta Smatanova from the University of South Bohemia, Czech Republik. Successful crystallization of biological macromolecules depends on the purification process and the crystallization methodology; on the balance of the large number of variables in solution composition and final purity of the protein are critical. The book provides a mathematical-physical interpretation of crystallization, with an improved theoretical insight into the processes of nucleation and crystal growth.

Watson Fuller, Keele University, UK, reviewed the book ‘Unravelling the double helix: the lost heroes of DNA’ written by Gareth Williams, issued in London in 2019 by Weidenfeld & Nicholson. The book is not only about the science behind the DNA story but also about the participants over about one hundred years from the mid decades of the nineteenth century in the context of the changing social and political milieu.

Guatam R. Desiraju from the Indian Institute of Science, Bangalore gives an overview of the book ‘The Hydrogen Bond. A Bond for Life’ by Aloys Hüttermann, published by De Gruyter in 2019 in Berlin. Early college students are aimed at this book. The former list of such books on the topic mostly concentrates on water, but this one describes the hydrogen bond as ‘the choice for life processes, an interaction that is not too weak, not too strong, not too stable, not too unstable, can be made and broken just as easily’. The reader of the book review gets an additional lesson on how to create analogies considering socio-cultural aspects, and to be accurate avoiding oversimplification or tedious details.


Just around the days that the review of the book ‘The Rhubarb connection and other revelations: the everyday world of metal ions’ by Lars Öhrström and Jacques Covès, published by the Royal Society of Chemistry in 2019 from Carla Pretorius, Stellenbosch University SA, was published on-line by Crystallography Reviews, Lars Öhrström visited my home institution and delivered a talk on his book. Being a professor of inorganic chemistry by himself he presented a fascinating history of some of the elements and small biomolecules including crystallographic aspects. There were interesting facts, sometimes romantic stories underlined by chemistry principles. A lecture like this – and the book for sure – catches the attention of the audience/the reader working in the field of the natural sciences, and may also recruit new, untrained people to be captivated with chemistry.

As ever we welcome new ideas for review articles, and for suggestions regarding books to be reviewed. Please contact me at the e-mail address below.

We look forward to welcoming your submissions.

## References

- [1] Urzhumtsev AG, Lunin VY. Introduction to crystallographic refinement of macromolecular atomic models. *Crystallogr Rev.* 2019;25:164–262.
- [2] Franklin R. Testing aspherical atom refinements on small-molecule data sets. *Nature.* 1950;A34:909–921.
- [3] Henn J. Metrics for crystallographic diffraction- and fit-data: a review of existing ones and the need for new ones. *Crystallogr Rev.* 2019;25:83–156.

Petra Bombicz  
*Research Centre for Natural Sciences*  
 [bombicz.petra@ttk.hu](mailto:bombicz.petra@ttk.hu)