Computational methods in macromolecular crystallography

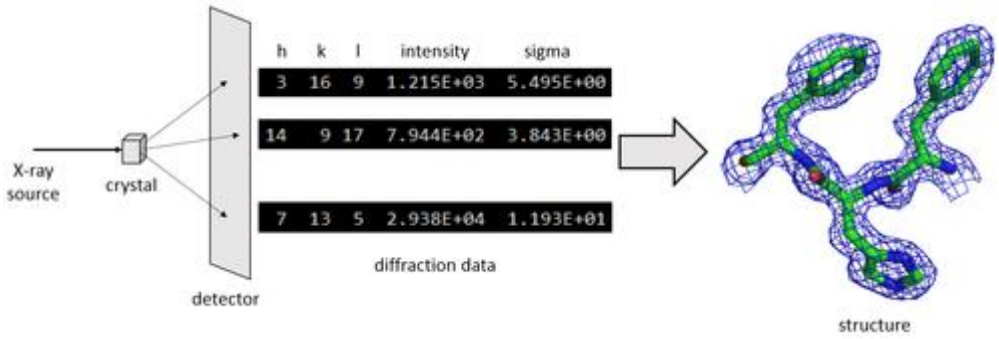
Single crystal X-ray diffraction is a robust method for determination of structures of macromolecules. Understanding of structures of biolically important macromolecules and their complexes help understand cellular processes, immune system processes, and desing novel biotechnologies.

As well as many other methods, macromolecular crystallography is being constantly developed. Dramatic improvement can be observed in experimental setup, but also in data processing and interpretation. Our laboratory is focused on development of software tools.

Current topics:

- **Identification of weakly bound ligands in macromolecular structures.**
- **Analysis and scaling of anisotropic data.**

Furthermore, we would like to work on updates of program **PAIREF** that helps users to perform **paired refinement** automatically.



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