# X-Ray Crystallography Resources

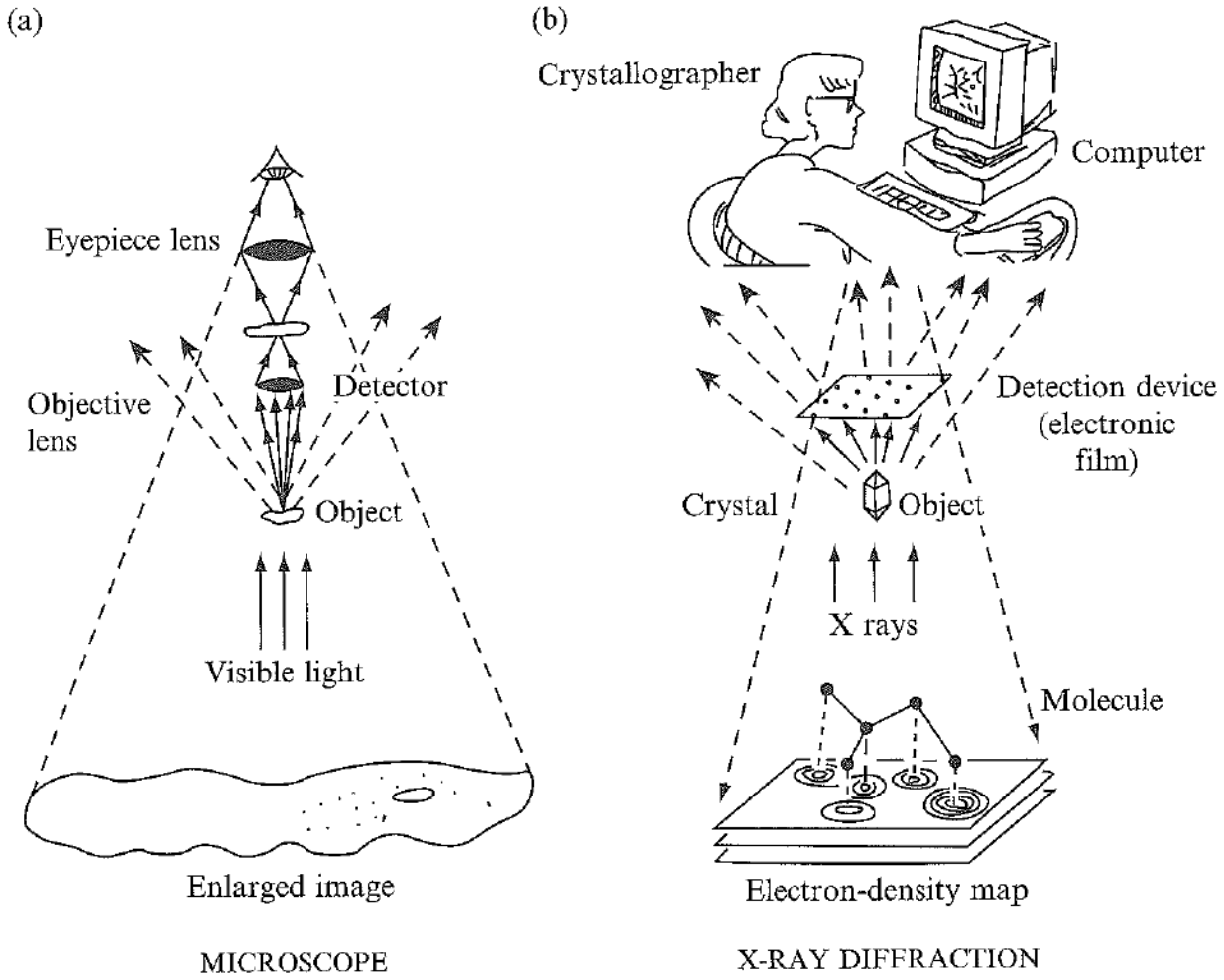
- Cantor and Schimmel, Chapter 13
  - Good, mathematical but dated
- Eisenberg and Crothers, Chapter 17
  - Good but also old
- Glusker and Trueblood, *Crystal Structure Analysis: A Primer*
  - Very good introductory text
- Rhodes, *Crystallography Made Crystal Clear*
  - Short text, intended for end users (not crystallographers)
- Blundell and Johnson, *Protein Crystallography*
  - Classic text, but very old at this point
- Rupp, *Biomolecular Crystallography*
  - Maybe a modern replacement for Blundell and Johnson?

Beyond the scope of this course

# X-Ray vs. NMR

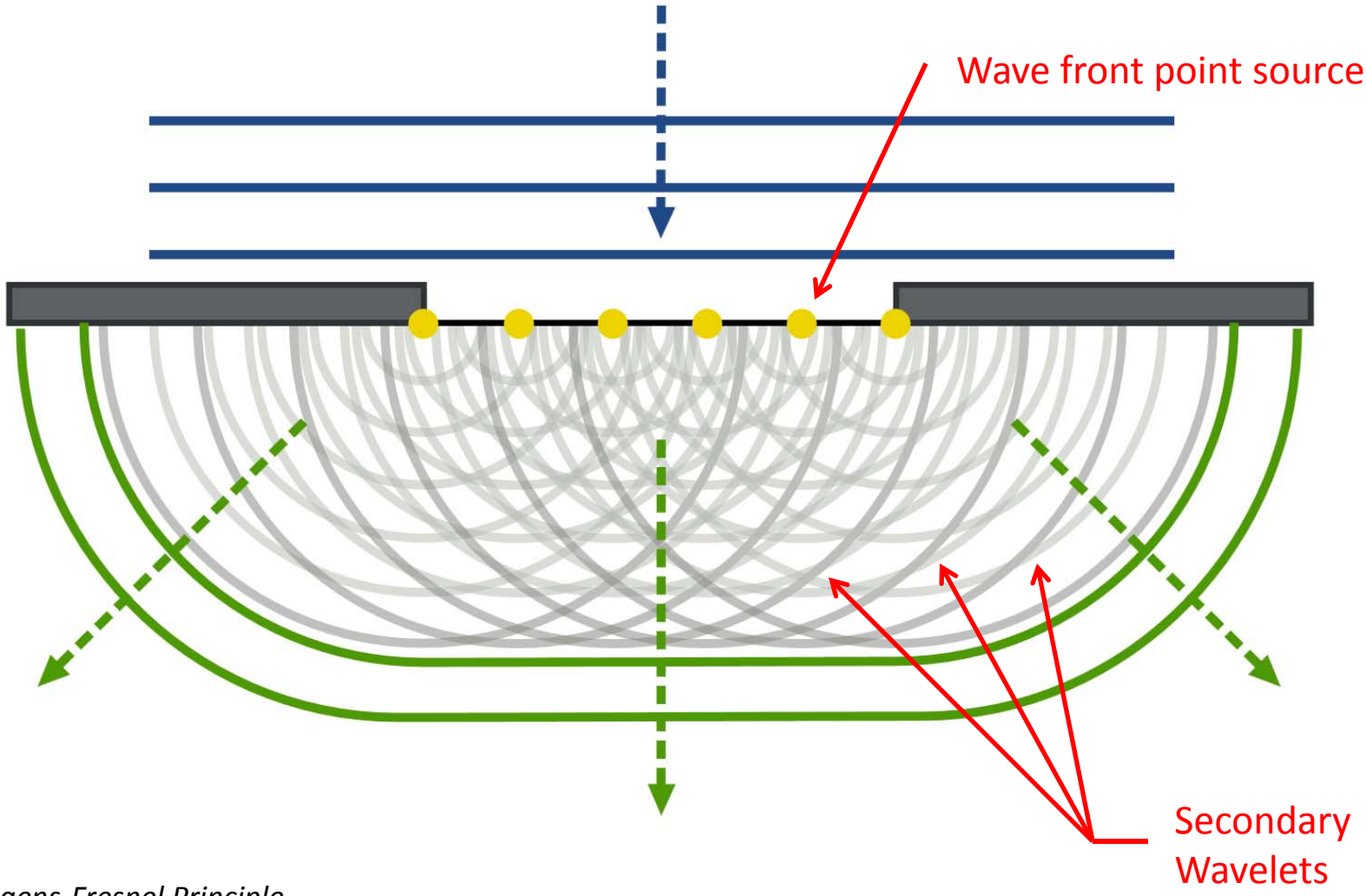
| X-Ray Crystallography | NMR Spectroscopy |
| --- | --- |
| Pros<br>• Large complexes<br>• Highly accurate structures | Pros<br>• Dynamics + structure<br>• Detect changes in solution state |
| Cons<br>• Crystal conditions<br>• Static structures | Cons<br>• Solution conditions<br>• Less accurate structures<br>• Size limited (but getting better) |

# Crystallography vs. Microscopy




From *Crystal Structure Analysis: A Primer*
Glusker & Trueblood, Chapt. 1, p. 5

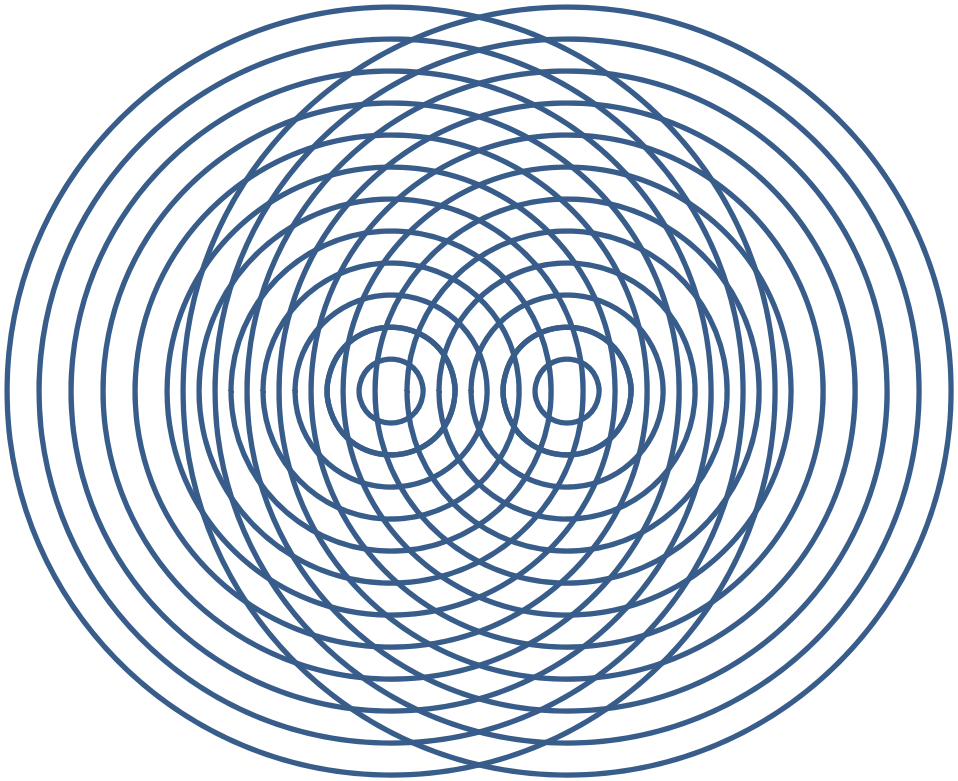
# Huygens-Fresnel Principle




From *Huygens-Fresnel Principle*
http://en.wikipedia.org/wiki/Huygens-Fresnel_principle

# Resolution and Wavelength

- As point sources become closer (less than λ), it becomes harder to see diffraction.
- Limit of resolution is approximately λ/2
- X-rays required to resolve bond lengths



λ

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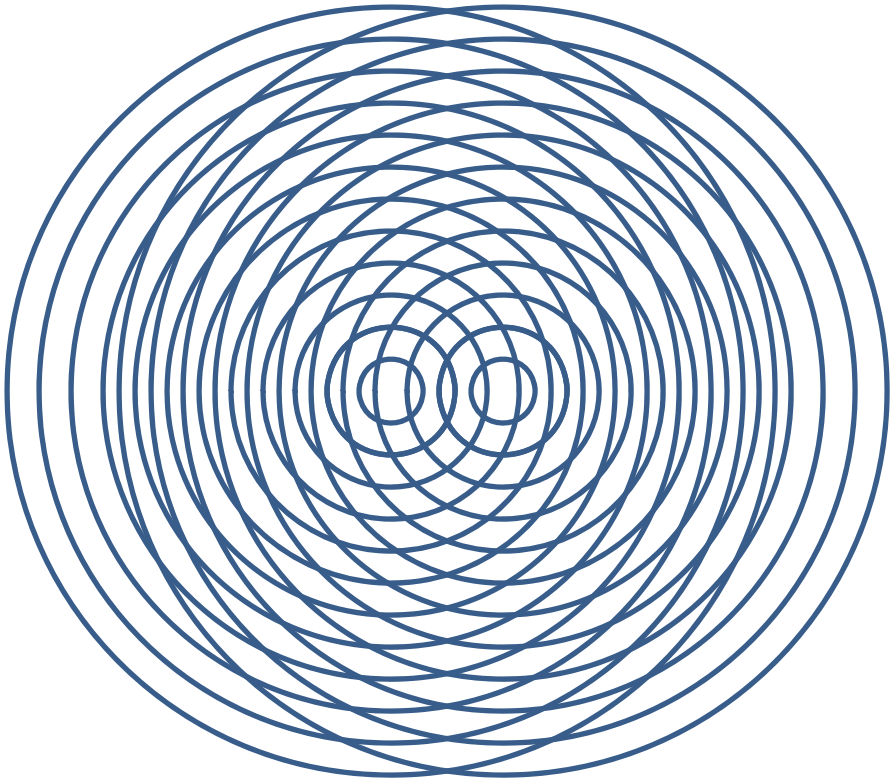

λ

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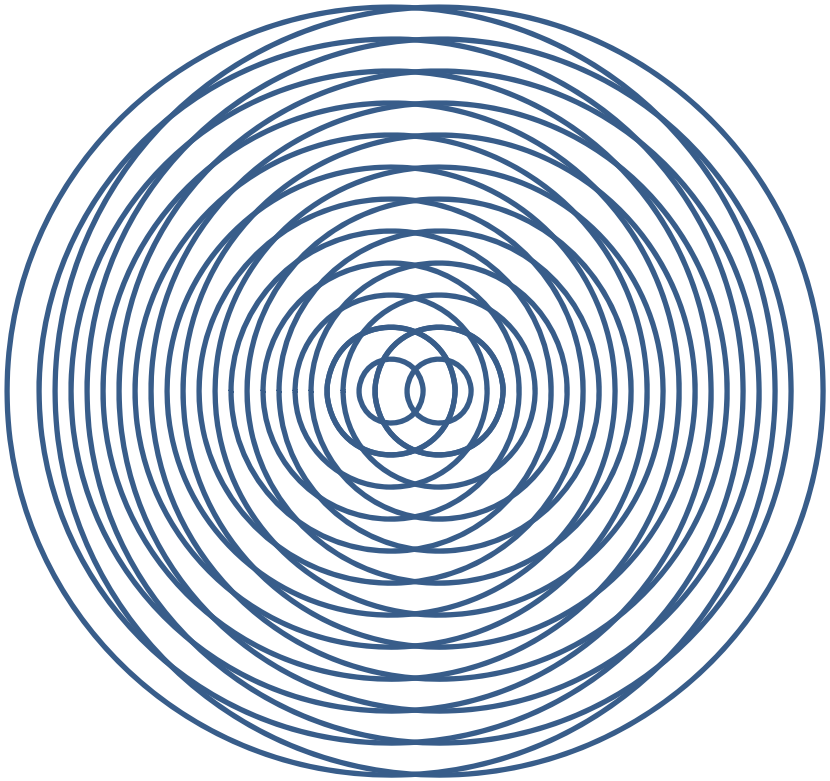

λ

# Resolution and Wavelength

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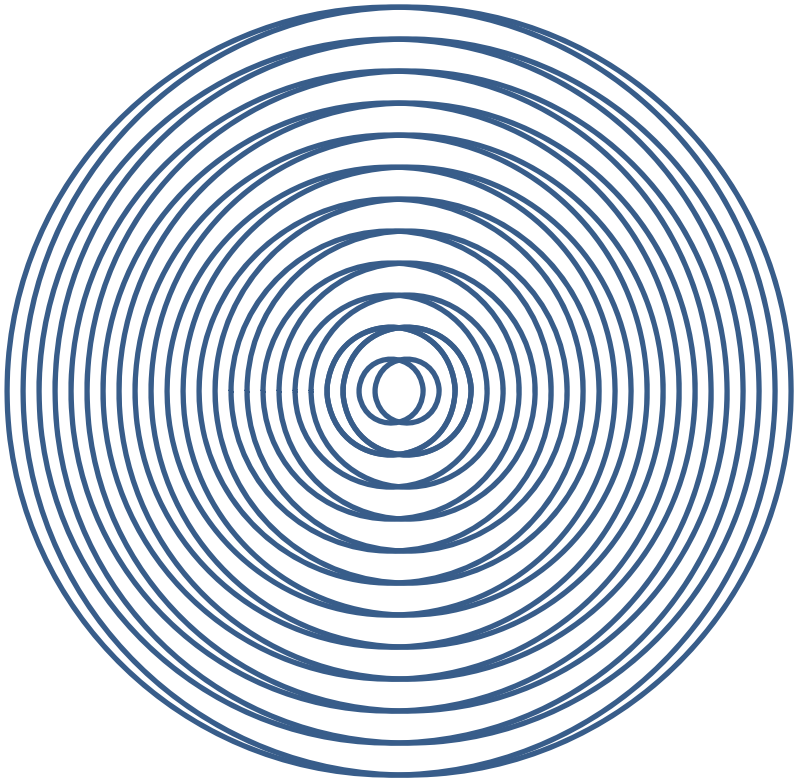
- X-rays required to resolve bond lengths (1-2 Å)

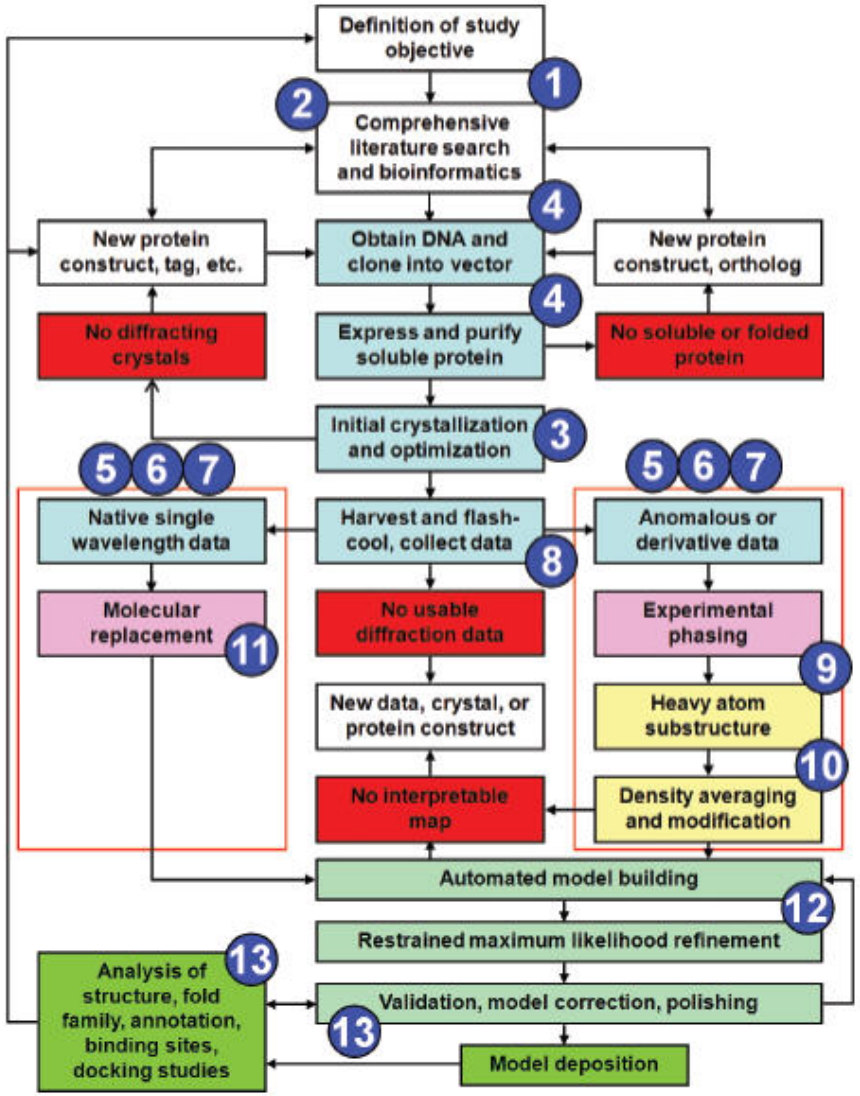


λ

# Crystallography Flow Chart

**Figure 1-8 Key stages in the structure determination process.** The flow diagram provides an overview of the major steps in a structure determination project, labeled with the chapter numbers treating the subject or related general fundamentals. Blue shaded boxes indicate experimental laboratory work, while all steps past data collection are conducted *in silico*. Protein production is discussed in Chapter 4, once we understand the process of crystallization and the requirements a protein must meet to be able to crystallize (Chapter 3).

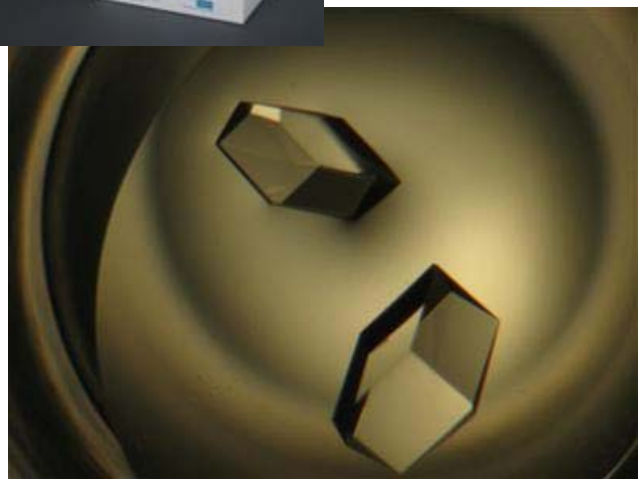





From *Biomolecular Crystallography* Rupp, Chapt. 1.

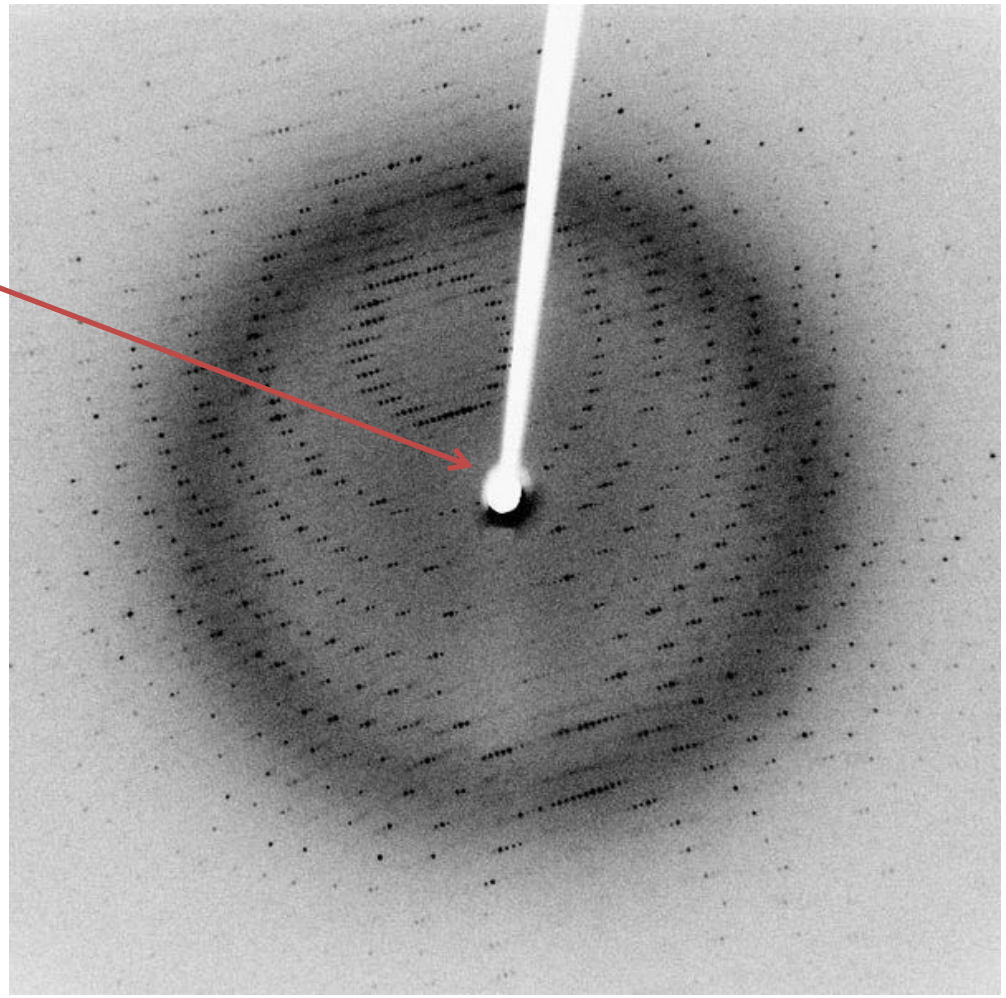
# Crystal Screens

- High-quality buffers and established precipitants
- Standardized, and (mostly) reproducible
- What if it doesn't work?

(lysozyme)

# Data Collection




From *Diffraction*
http://en.wikipedia.org/wiki/Diffraction

# Summary

- Electrons diffract X-rays: more electrons means a stronger interaction
- X-rays probe distances on the order of their wavelengths (~1 Å)
- Many steps required for structure refinement
- Protein crystals require meticulousness, good biochemistry, and little luck
- Result: electron density map, can fit atoms into density