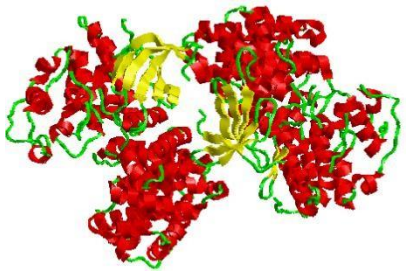
X-ray crystallography: understanding protein structures

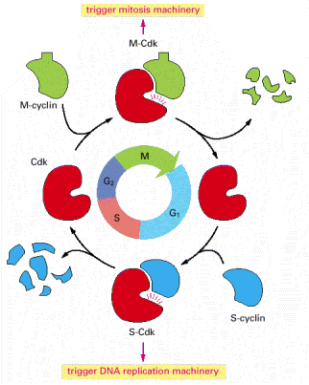
Proteins play a variety of fundamental roles in life processes:
- there are structural proteins
(for example the horny outer layer of human and animal skin and proteins of the cytoskeleton)
- proteins that catalyze chemical reactions (enzymes)
- transport and storage proteins (haemoglobin, ferritin)
- regulatory proteins, including hormones and receptor/signal transduction proteins
- proteins that control gene transcription
- and proteins involved in recognition, such as antibodies and proteins of the immune system

We derive our understanding of protein functions from protein structures resolved at the atomic detail.

The amino acid sequence of a protein dictates its three dimensional structure.
The functions of proteins depend on their adopting native three dimensional structure.

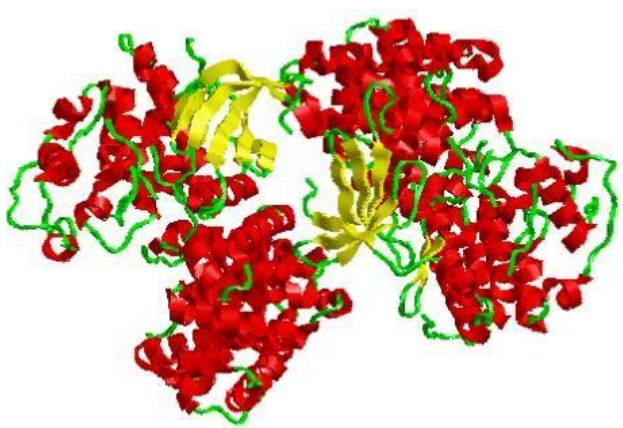
MENFQKVEKI GEGTYGVVYK ARNK
LTGEVV ALKKIRLDTE TEGVPSTAIR
EISLLKELNH

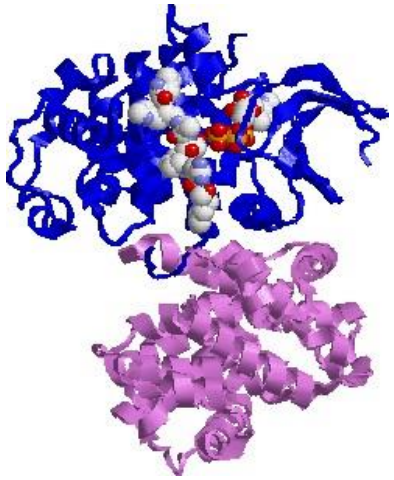


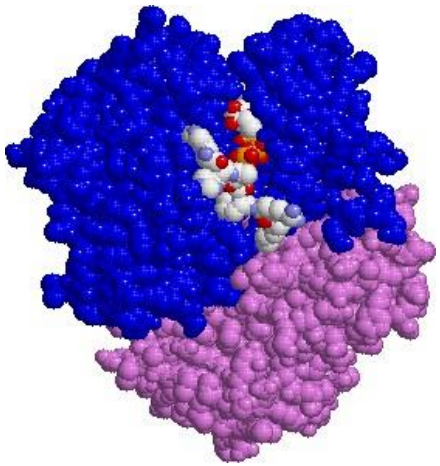


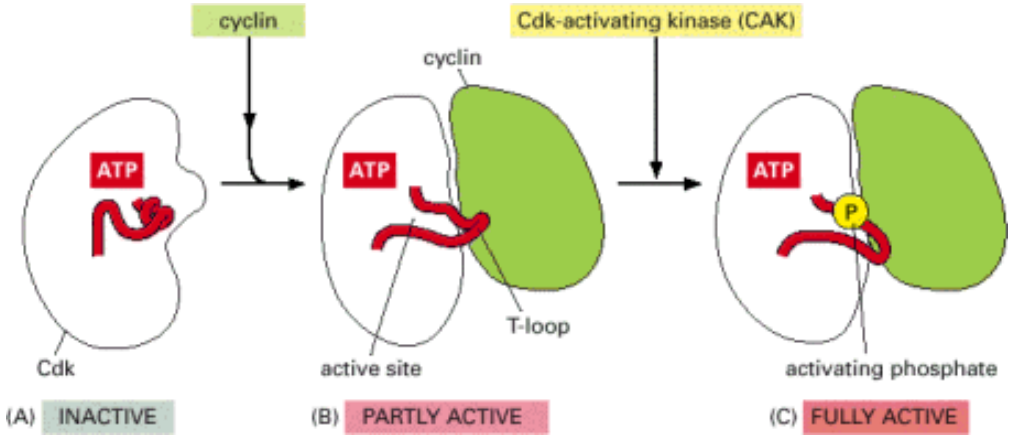
An example…

The native structure of an enzyme may have a cavity in its surface that binds a small molecule and juxtaposes it to catalytic residues.
PHOSPHORYLATED CDK2-CYCLYIN A-SUBSTRATE PEPTIDE COMPLEX







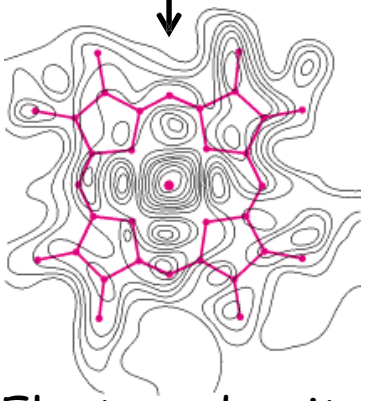


Steps in protein crystallography

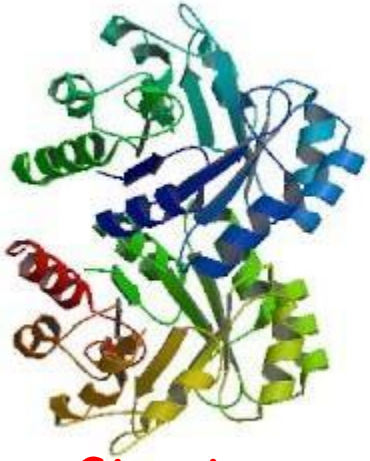
Purified protein

Crystal

Data collection



Electron density

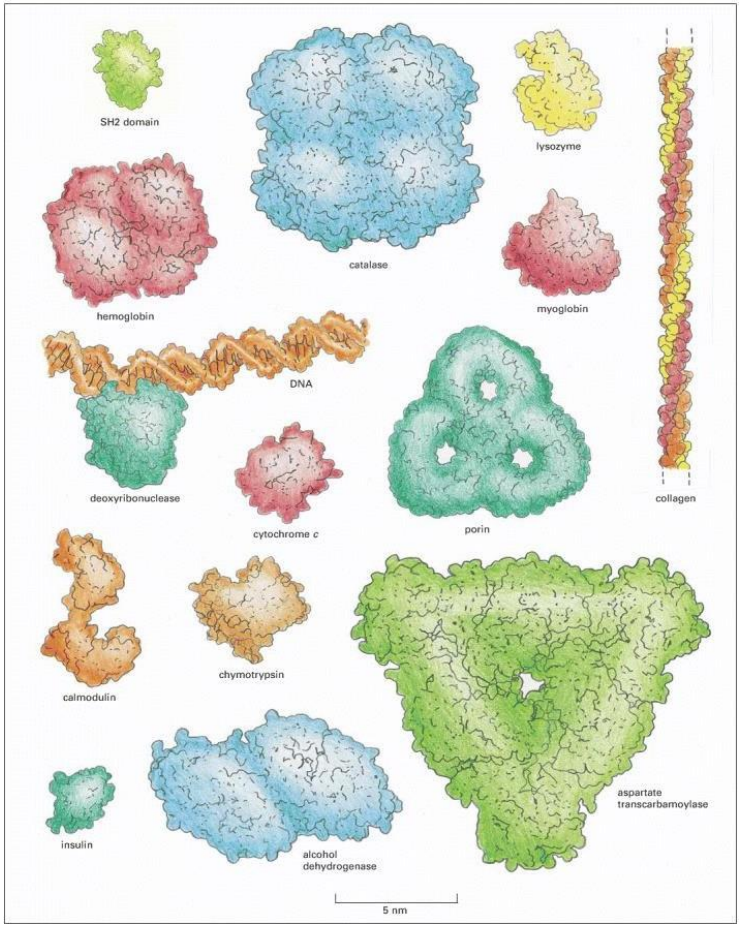


Structure

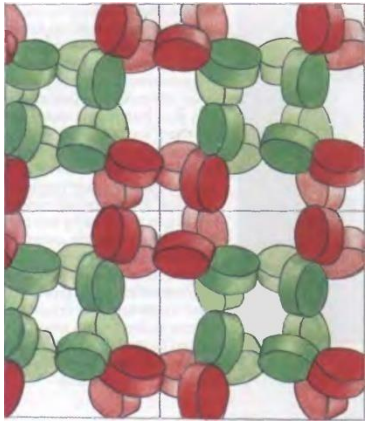
Protein crystals are difficult to grow

Without crystals there can be no X-ray structure determination of a protein!

you need a regular cristal to have a good resolution



=

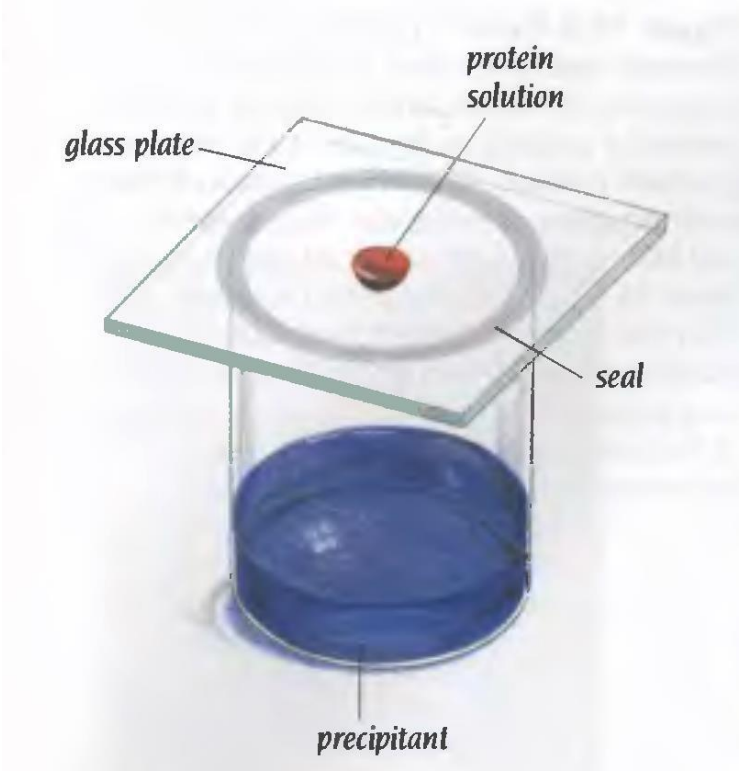


A crystal is a three-dimensional regular structure formed by many identical molecules.

Proteins are large objects with irregular shapes and it is impossible to pack them into a crystal without forming large holes or channels between the individual molecules.

Growing crystals: the hanging drop method

the solution must be saturated to form a cristal



The formation of a crystal strongly depends on a number of different parameters, such as pH, temperature, protein concentration….

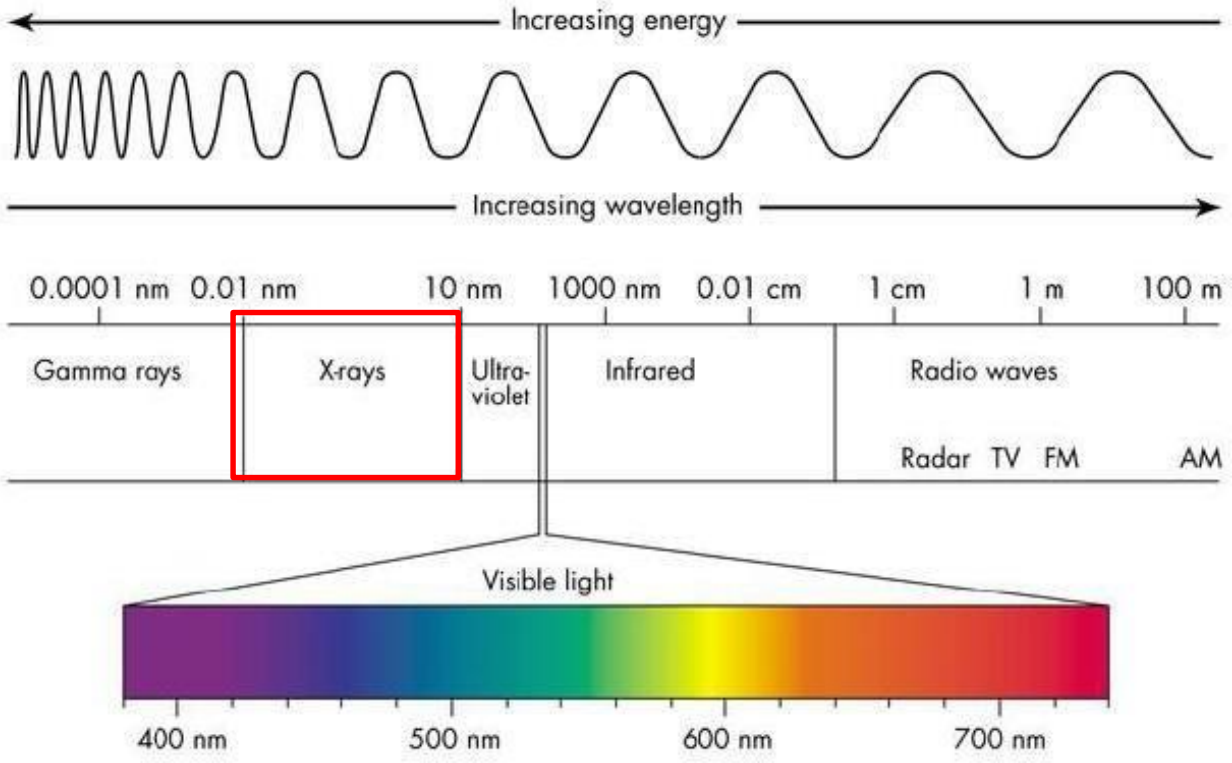
Well ordered protein crystals diffract X-rays.

Why X-rays?

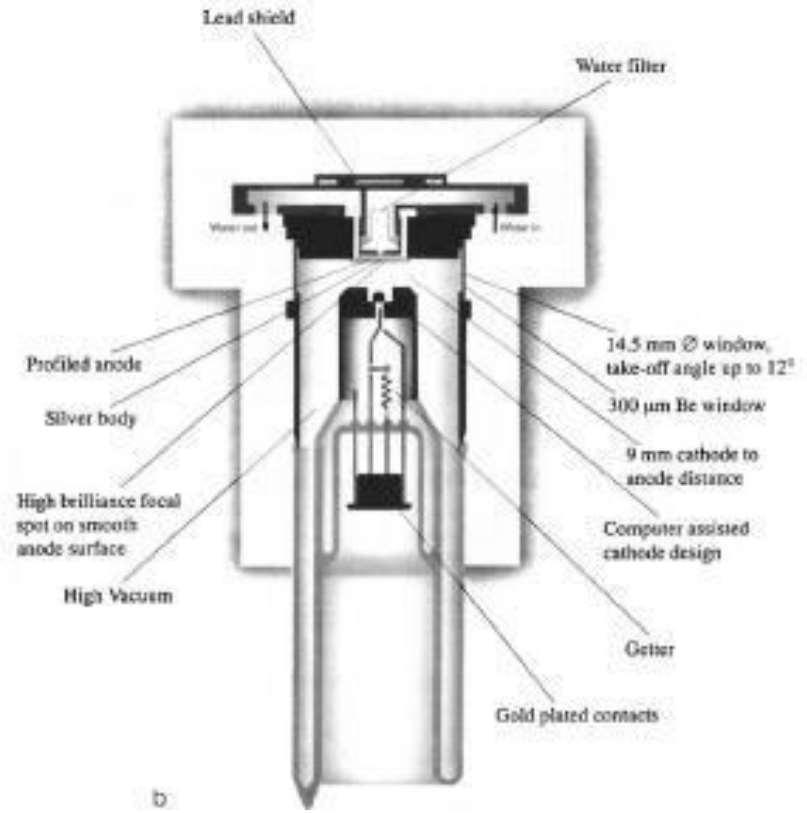
In order to measure something accurately you need the appropriate ruler.

The X-rays wavelength (typically between 10^{-11} and 10^{-8} m)
[10 Å and 0.01 Å] has the same order of magnitude of a covalent bond.

The type of X-rays used by crystallographers are ~ 0.5 to 1.5 Å long.



Obtaining X-rays: rotating anode tube



Within a high voltage tube a cathode emits electrons. Because the tube is under vacuum and the cathode is at high negative potential with respect to a metal plate (anode), the electrons are accelerated and reach the anode at high speed.

Most of the energy is converted to heat. The anode can be a rotating cylinder.

Obtaining X-rays: the synchrotron

It is a supermicroscope:
it is capable of resolving the structure of matter down to the level of atoms and molecules.

X-rays are the emission of accelerated charged particles moving in a magnetic field.

http://www.esrf.eu/AboutUs/GuidedTour/Anim2

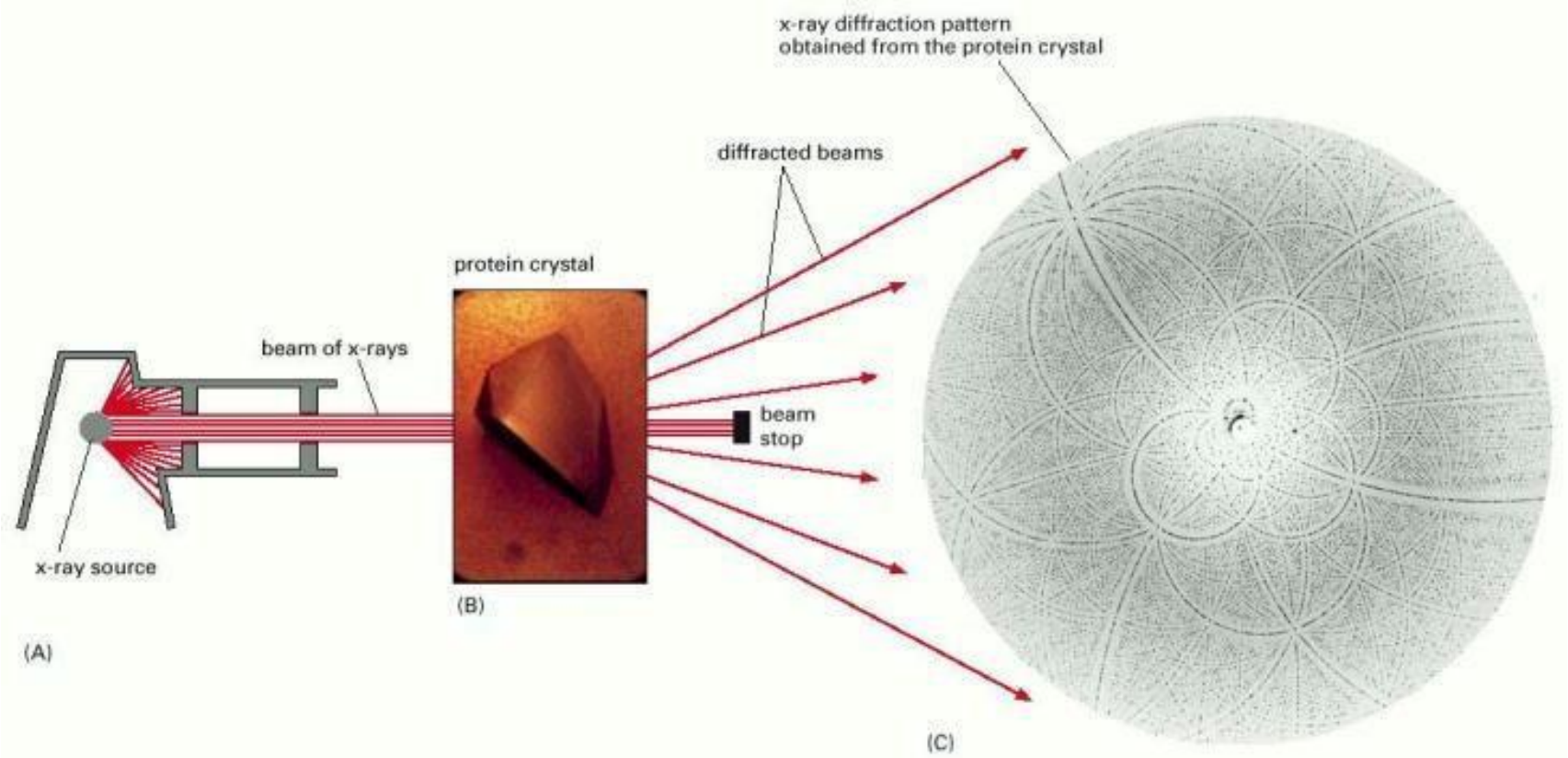
The three largest and most powerful synchrotrons in the world

APS, Usa

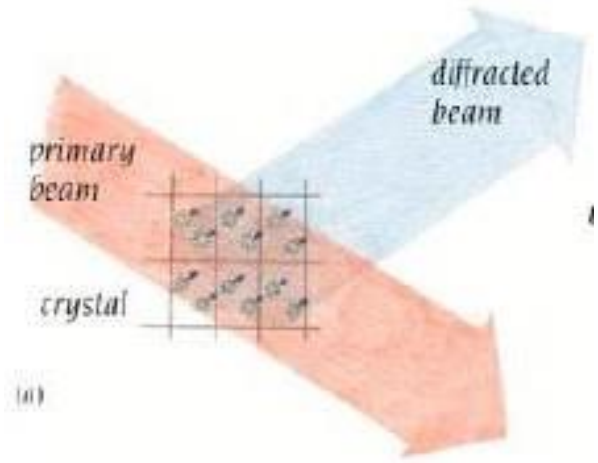
ESRF
Europe-France

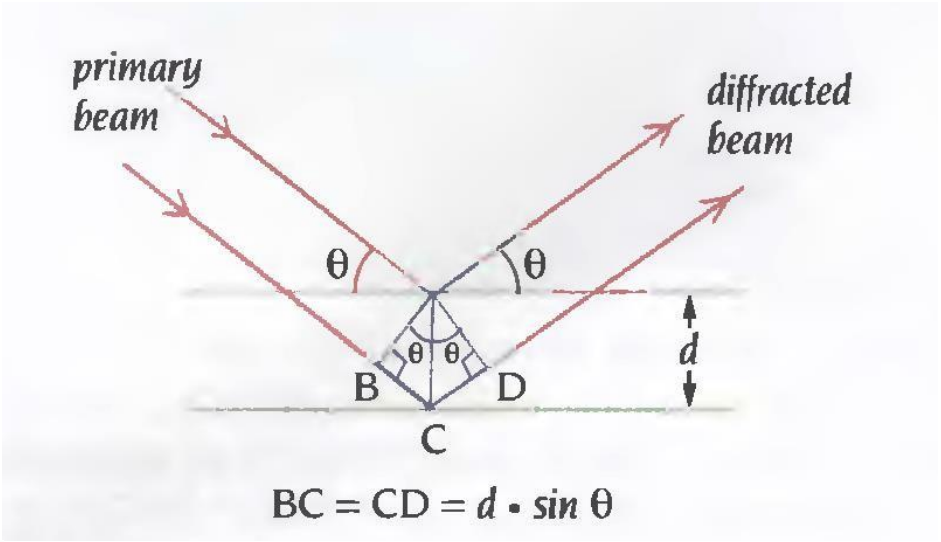
Spring-8, Japan

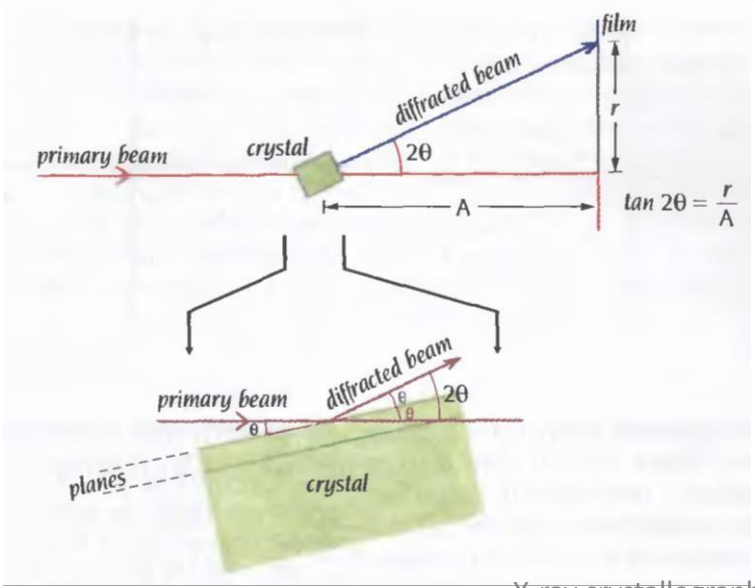
The experiment



The Bragg's law for diffraction







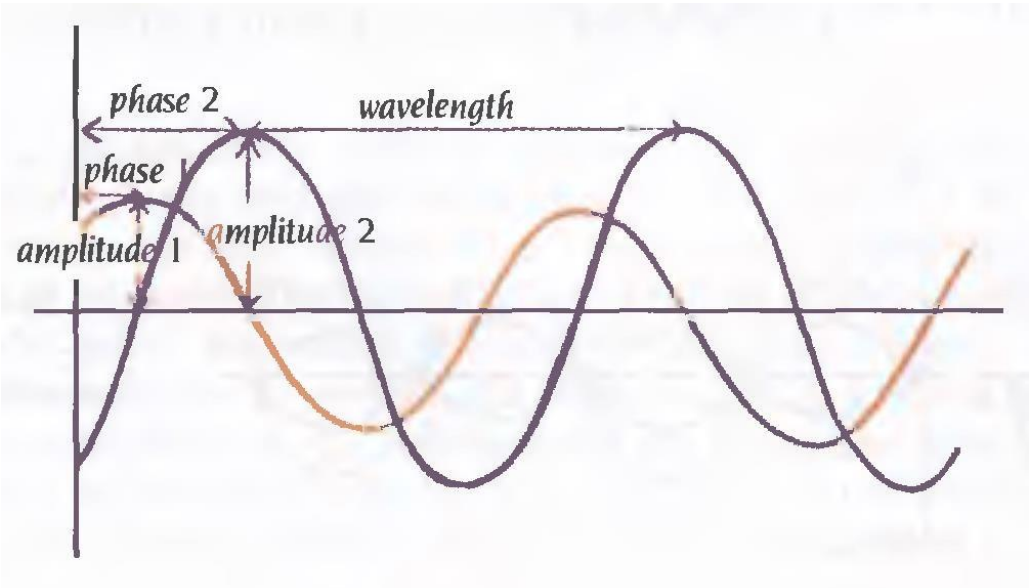
X-rays reflected from the lower plane travel a farther distance of BC+CD

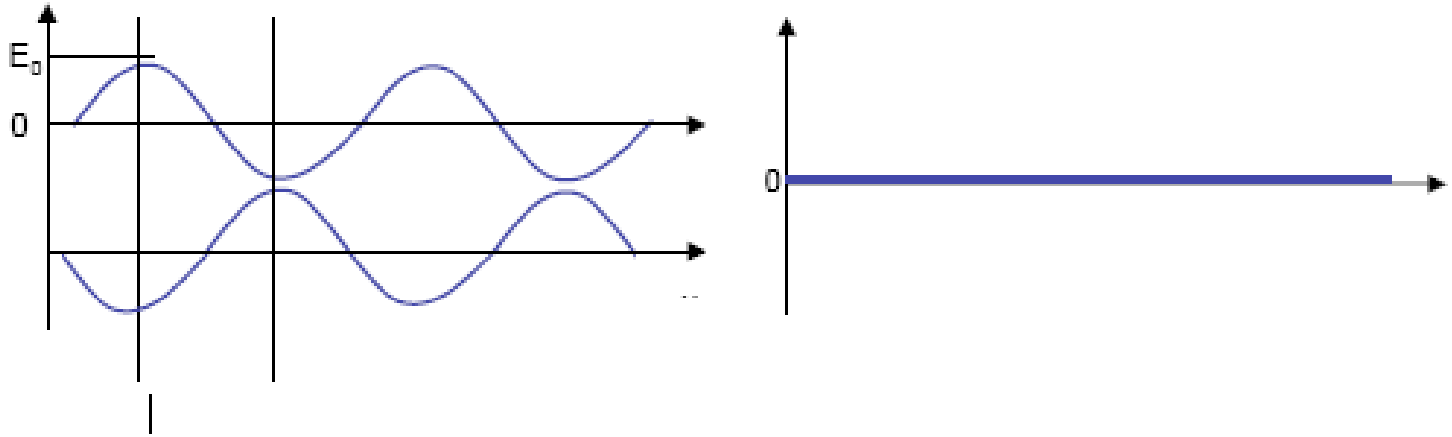
$BC+CD = 2d \sin\theta$

We observe a reflected wave only if this distance is equal to an integer number of the wavelength λ.

Bragg's law for diffraction: $2d \sin\theta = n\lambda$

Wave basics

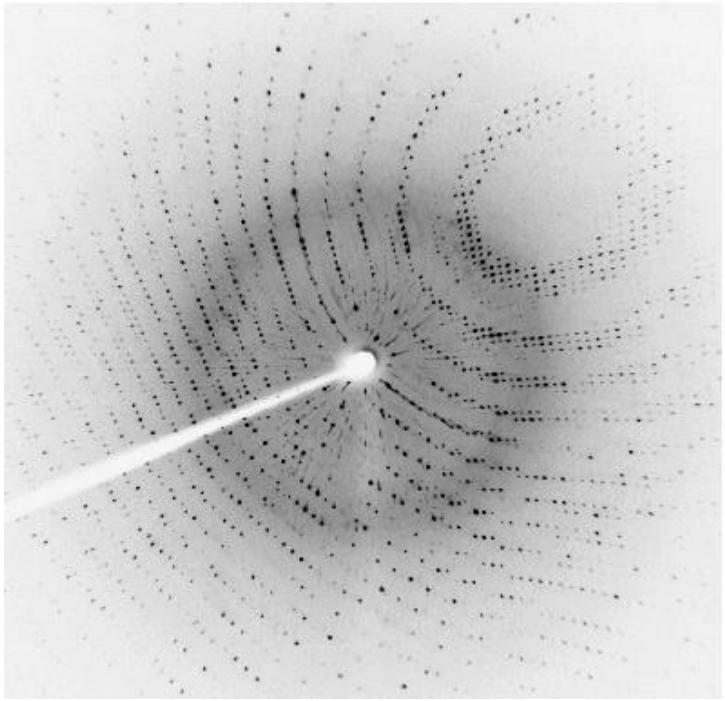




Destructive interference

Extract the information

Each atom in a crystal scatters X-rays in all directions. Only those that positively interfere with one another, accordingly to the Bragg's law, give rise to diffracted beams that are recorded as different diffraction spots.

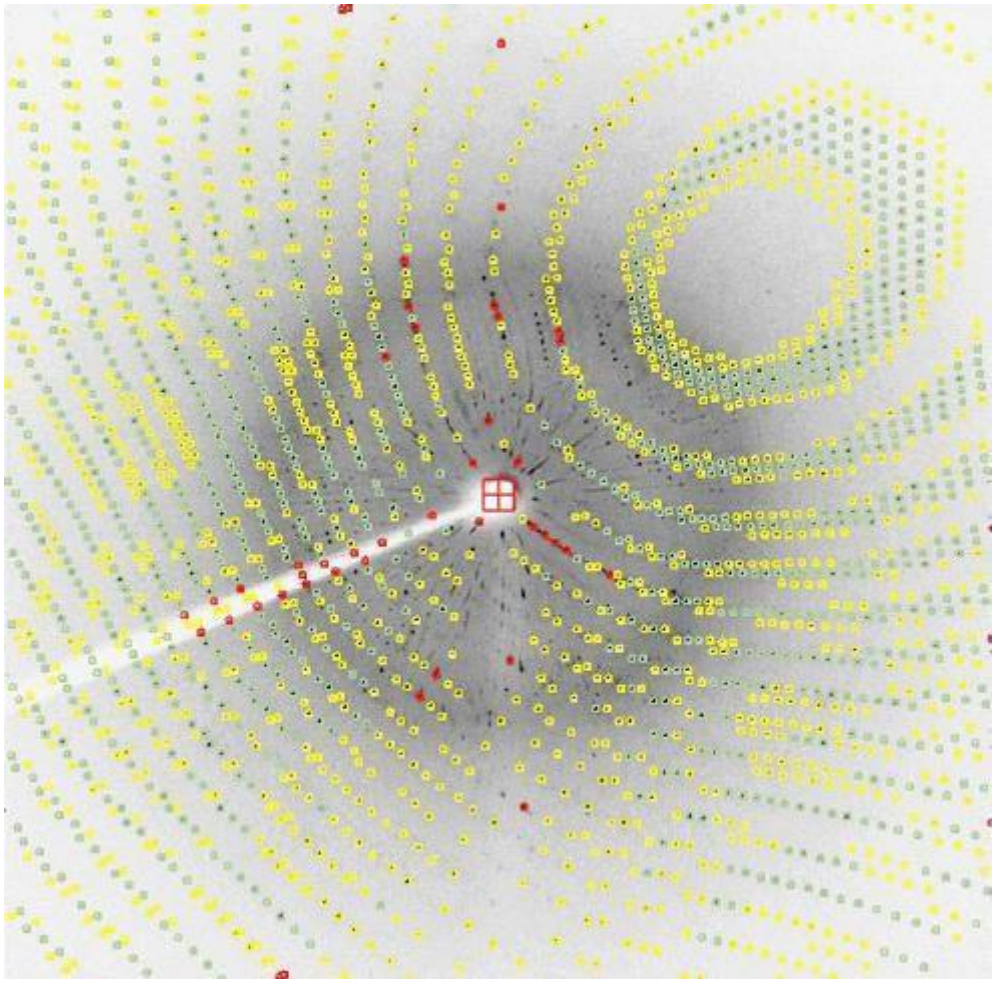


Each spot is the result of interference of all X-rays with the same diffraction angle emerging from all atoms.

In a typical protein crystal (myoglobin), each of the about 20000 diffracted beams measured contains scattered X-rays from each of the around 1500 atoms of the protein.

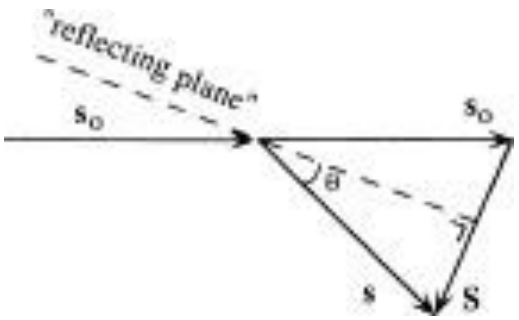
How can we extract information about individual atoms from such a system?

Data collection



H	K	L	I
-29	6	-12	220.4
-25	-4	-14	482.7
-30	13	-10	1012.2
-26	-1	-13	1069.2
-24	-5	-14	6299.6
-29	11	-10	1017.9
-29	10	-10	3558.4
-25	-3	-13	22.0
-23	-6	-14	7385.6
-29	15	-9	226.4
-26	0	-12	271.8
-29	14	-9	2370.3
-29	13	-9	396.2
-29	20	-8	1108.8

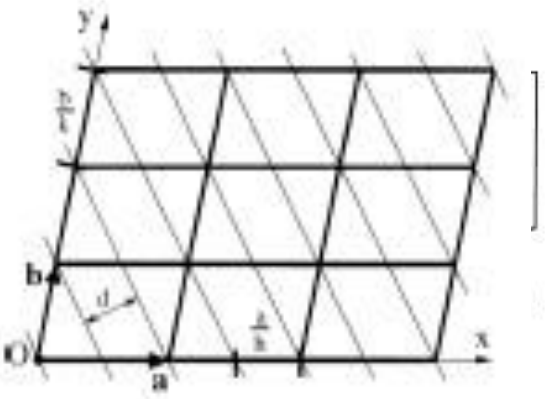
Bragg's interpretation



The wave can be regarded as being reflected against a plane with θ as the reflecting angle and $\vec{S}$ is perpendicular to the "imaginary relfecting plane".

$$|S| = 2(\sin A)/Z$$

This planes split the *x*-axis in a/h pieces, the *y*-axis in b/k pieces and the *z*-axis in c/l pieces. A set of lattice planes is thus determined by three indices h,k,l. The projection of a/h, b/k and c/l on the line perpendicular to the corresponding lattice plane is equal to the distance d between the planes.



All the planes with $\vec{r} \bullet \vec{S}$ equal to an integer are reflecting in phase and form a series of Bragg planes.

$$\frac{1}{|S|} = d \quad |S| = 2(\sin A)/Z \longrightarrow \frac{2d(\sin A)}{Z} = 1$$

Calculating the electron density: Fourier transform

$$\vec{F}(\vec{S}) = \sum_{j=1}^{n} f_j \exp(2\pi i \vec{r}_j \bullet \vec{S})$$

Instead of summing over all separate atoms , we can integrate over all electrons in the unit cell

$$\vec{F}(\vec{S}) = \int_{cell} \theta(r) \exp(2\pi i \vec{r} \bullet \vec{S}) dv$$

where $\theta(r)$ is the density at position **r** at the unit cell.

If *x,y* and *z* are fractional coordinates in the unit cell
($0 \le x \le 1$, the same for y and z) and V is the volume of the unit cell

$$dv = V \bullet dxdydz \qquad \vec{r} \bullet \vec{S} = (\vec{a} \bullet x + \vec{b} \bullet y + \vec{c} \bullet z) \bullet \vec{S} = a\vec{} \bullet \vec{S} \bullet x + b\vec{} \bullet \vec{S} \bullet y + c\vec{} \bullet \vec{S} \bullet z$$

$$= hx + ky + lz$$

$$\vec{F}(hkl) = V \int_{x=0}^{1} \int_{y=0}^{1} \int_{z=0}^{1} \theta(x, y, z) \exp[2\pi i(hx + ky + lz)] dxdydz$$

Calculating the electron density: Fourier transform

The goal of X-ray crystallography is NOT to calculate the diffraction pattern BUT to calculate the electron density at every position *x,y,z* in the unit cell.

This can be done by Fourier transformation.

$$\vec{F}(hkl) = V \int_{x=0}^{1} \int_{y=0}^{1} \int_{z=0}^{1} \theta(x, y, z) \exp[2\pi i(hx + ky + lz)] dx dy dz$$

$\vec{F}(hkl)$ is the Fourier transform of $\theta(x, y, z)$ but the reverse is also true: $\theta(x, y, z)$ is the Fourier transform of $\vec{F}(hkl)$

$$\theta(x, y, z) = \frac{1}{V} \sum_{h} \sum_{k} \sum_{l} \vec{F}(hkl) \exp[-2\pi i(hx + ky + lz)]$$

Laue conditions tell us that diffraction occurs only in discrete directions and for this reason the integration can be replaced by a summation.

Calculating the electron density: the phase problem

OLD PROBLEM

The Fourier transform provides a mathematical correspondence between two physical spaces: one we wish to know about (molecular structure) but not directly accessible to us, and another in which measurements are made.

$$\theta(x,y,z) = \frac{1}{V}\sum_h \sum_k \sum_l \vec{F}(hkl)\exp[-2\pi i(hx+ky+lz)]$$

because $\vec{F} = |F|\exp(i\alpha)$

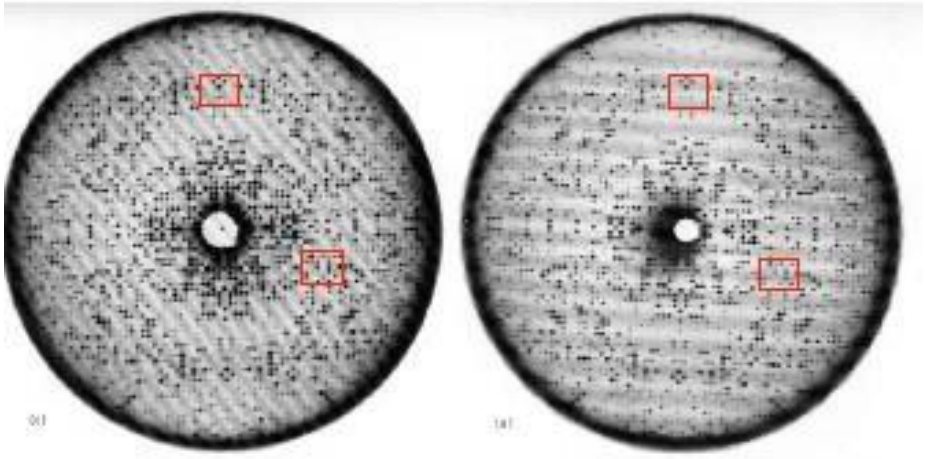
$$\theta(x,y,z) = \frac{1}{V}\sum_h \sum_k \sum_l |F(hkl)|\exp[-2\pi i(hx+ky+lz)+i\alpha(hkl)]$$

The intensity of a diffracted beam is proportional to the square of its amplitude, so we can obtain the $|F(hkl)|$ measuring the intensities of the spots.

The phase angles $\alpha(hkl)$ cannot be derived from the diffraction pattern.

A possible solution of the phase problem: the isomorphous replacement method

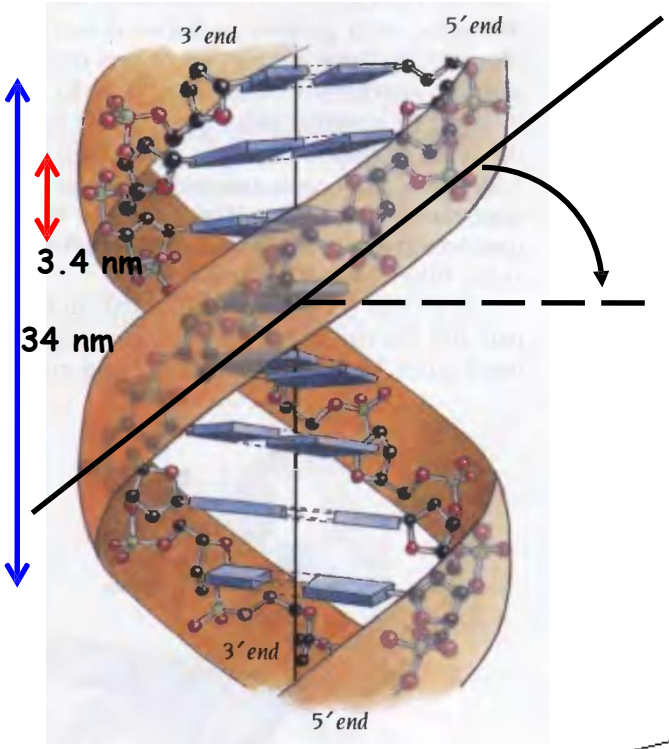
This technique requires the attachment of heavy atoms to the protein molecules in the crystal. These atoms scatter X-rays more strongly and they give a significant contribution to the diffraction pattern.

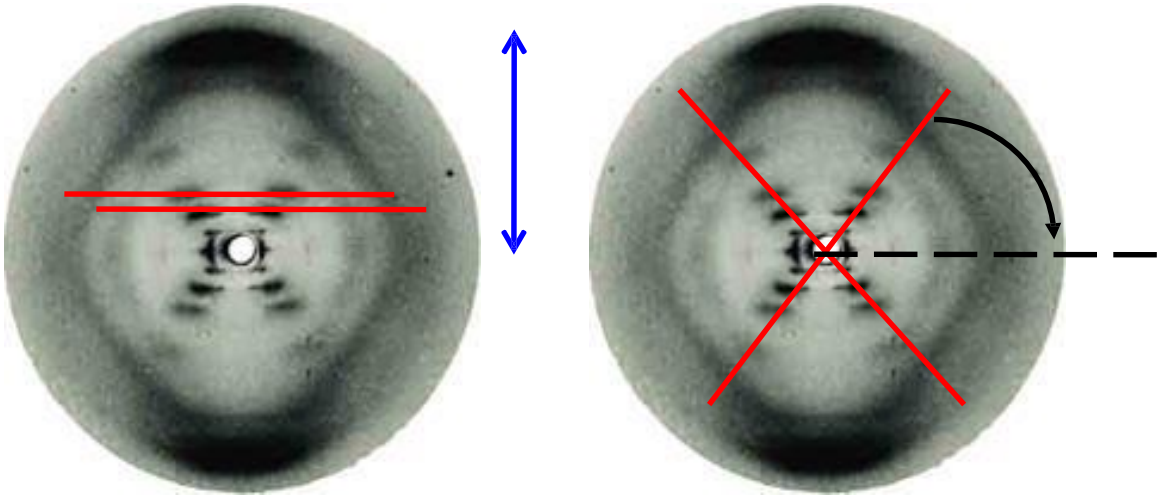


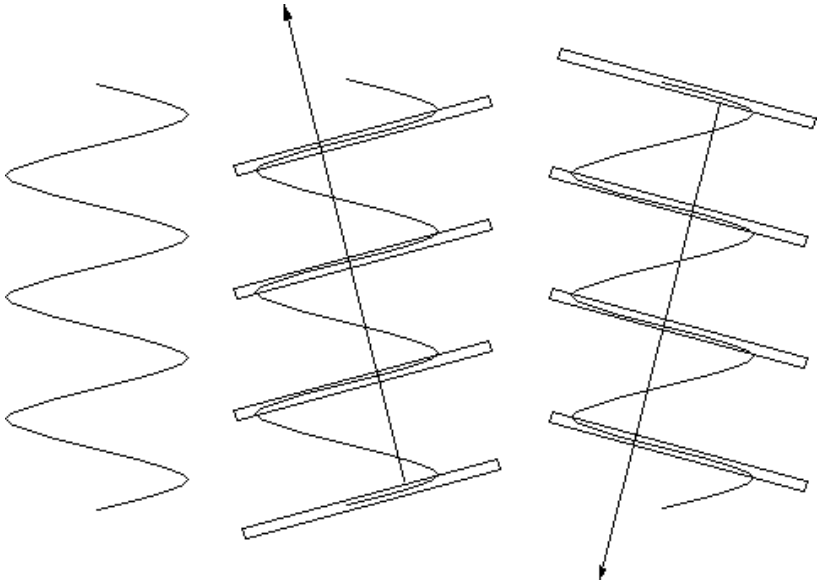
The intensity differences are used to deduce the heavy atoms positions in the unit cell. From the positions of the heavy atoms we can calculate the amplitudes and phases of their contributions to the diffracted beam.

We know the amplitude and the phase of the heavy atoms ,the amplitude of the protein alone and the amplitude of protein + heavy atoms: one phase and three amplitudes.

DNA diffraction pattern



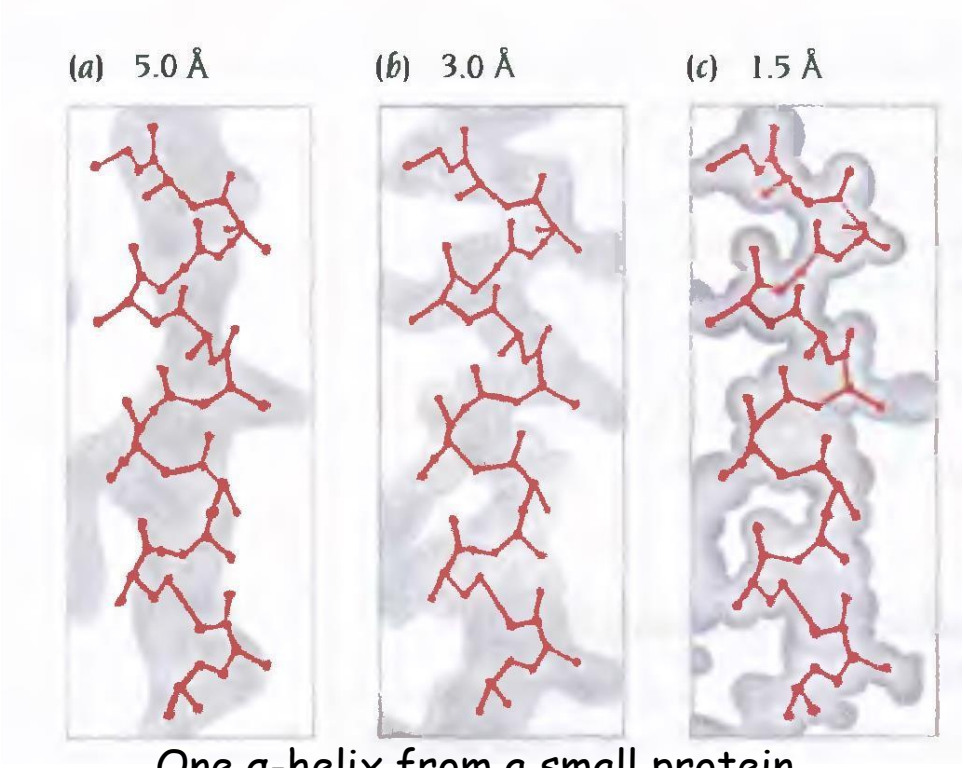




Building the model

RESOLUTION

Now the electron density map has to be interpreted as a polypeptide chain having a particular amino acid sequence.



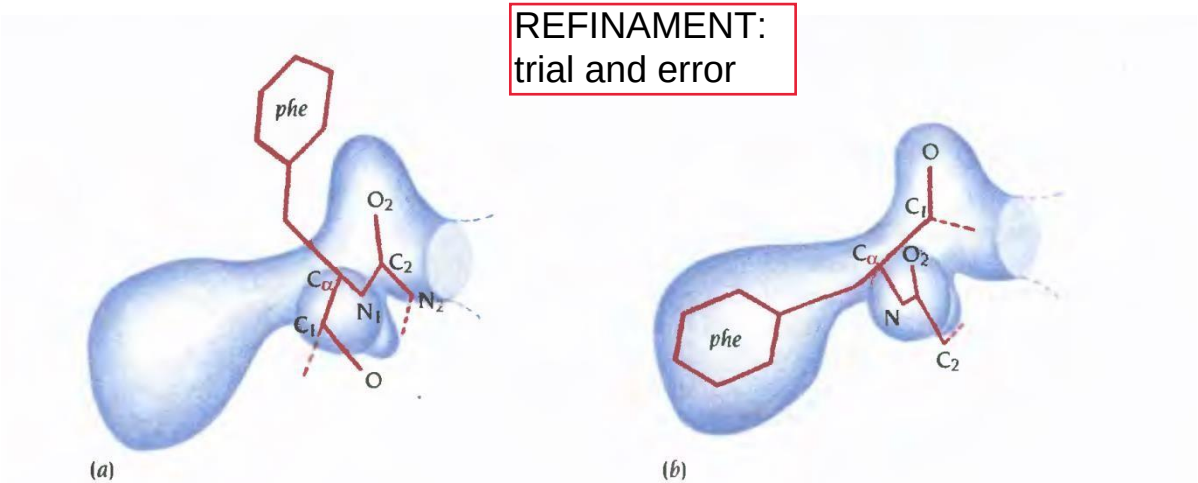
One α-helix from a small protein

This process is complicated because by several limitations of the data:
-the map contains errors, mainly due to errors in phase angles
-the quality of the map depends on the resolution of the diffraction data, which in turn depends on how well-ordered crystals are.

The resolution is measured in Å and it indicates the amount of detail that can be seen. The smaller the number is the great the resolution.

Building the model: trial and error

REFINAMENT:
trial and error



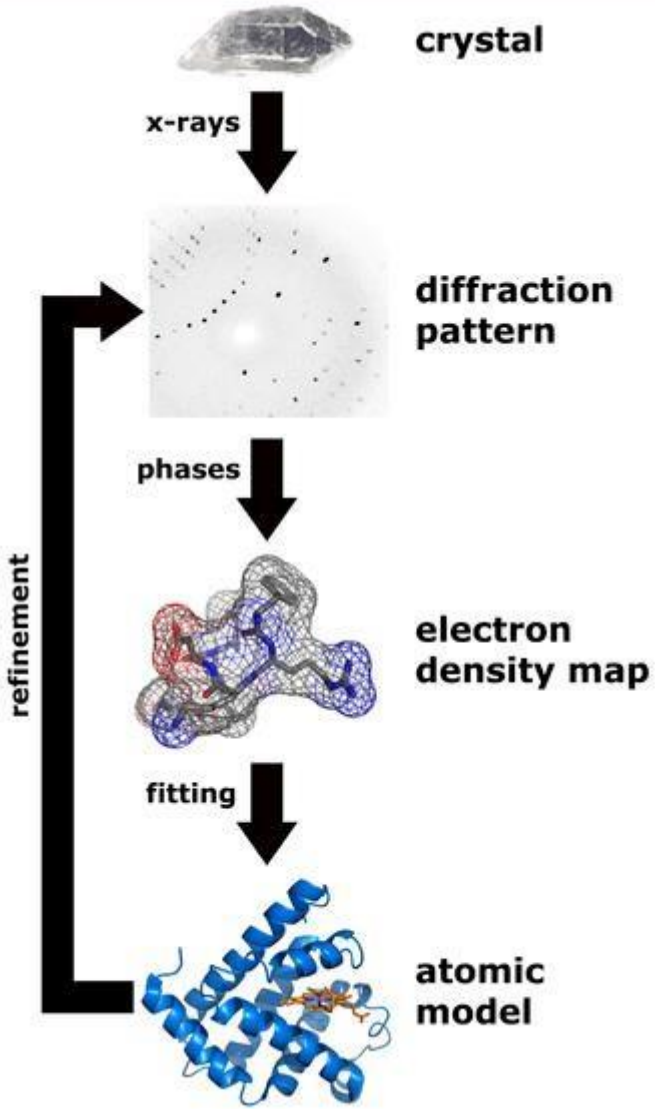
The electron density map is interpreted by fitting into it pieces of a polypeptide chain with known stereochemistry.

The units of the chain are initially arbitrarily orientated and then they can be rotated and translated relative to the electron density until a god fit is obtained.

This is not easy! A map showing continuous density from N-terminus to C-terminus is rare. A number of matches between the electron density map and discontinuous regions of the sequence are produced to build the model.

A refinement procedure removes errors from the model (provided high enough resolution, that is 2.5 Å or better).

SUMMING UP:


crystal
x-rays
diffraction pattern
phases
electron density map
fitting
atomic model
refinement

PDB file

```
HEADER    COMPLEX (PROTEIN KINASE/CYCLIN)          11-OCT-99   1QMZ
TITLE     PHOSPHORYLATED CDK2-CYCLYIN A-SUBSTRATE PEPTIDE COMPLEX
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: CELL DIVISION PROTEIN KINASE 2;
COMPND   3 CHAIN: A, C;
COMPND   4 SYNONYM: CYCLIN-DEPENDENT KINASE-2, CDK2, P33 PROTEIN
COMPND   5 KINASE;
COMPND   6 EC: 2.7.1.-;
COMPND   7 ENGINEERED: YES;
COMPND   8 OTHER_DETAILS: PHOSPHORYLATED;
COMPND   9 MOL_ID: 2;
COMPND  10 MOLECULE: G2/MITOTIC-SPECIFIC CYCLIN A;
COMPND  11 CHAIN: B, D;
COMPND  12 FRAGMENT: RESIDUES 174-432;
COMPND  13 SYNONYM: CCNA, CCN1;
COMPND  14 MOL_ID: 3;
COMPND  15 MOLECULE: SUBSTRATE PEPTIDE;
COMPND  16 CHAIN: E, F;
COMPND  17 FRAGMENT: 1-7

ATOM      1  N   SER A   0      30.751  78.499  13.070  1.00 56.01           N
ATOM      2  CA  SER A   0      31.820  77.511  13.078  1.00 57.14           C
ATOM      3  C   SER A   0      32.187  76.999  11.672  1.00 55.54           C
ATOM      4  O   SER A   0      33.420  76.858  11.379  1.00 56.80           O
ATOM      5  CB  SER A   0      31.586  76.367  14.057  1.00 58.43           C
ATOM      6  OG  SER A   0      32.344  76.601  15.261  1.00 60.79           O
ATOM      7  N   MET A   1      31.314  76.108  11.171  1.00 51.11           N
ATOM      8  CA  MET A   1      31.359  75.777   9.762  1.00 47.09           C
ATOM      9  C   MET A   1      30.736  76.955   9.022  1.00 45.17           C
ATOM     10  O   MET A   1      30.254  76.757   7.930  1.00 39.77           O
ATOM     11  CB  MET A   1      30.568  74.492   9.501  1.00 46.64           C
ATOM     12  CG  MET A   1      31.103  73.201  10.126  1.00 48.44           C
ATOM     13  SD  MET A   1      32.931  73.080   9.964  1.00 48.07           S
ATOM     14  CE  MET A   1      32.848  72.799   8.179  1.00 50.18           C
ATOM     15  N   GLU A   2      30.731  78.163   9.626  1.00 43.86           N
ATOM     16  CA  GLU A   2      30.057  79.281   8.983  1.00 44.38           C
ATOM     17  C   GLU A   2      30.589  79.578   7.591  1.00 40.48           C
```

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB Login

RCSB PDB PROTEIN DATA BANK

135201 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands

Go

Advanced Search | Browse by Annotations

PDB-101 wwPDB EMDataBank NDB NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation

Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

A Structural View of Biology

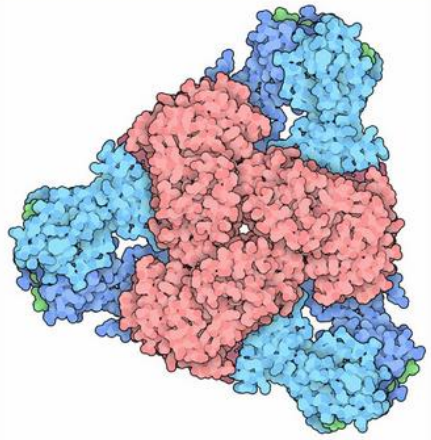
This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

Video: How Enzymes Work

November **Molecule of the Month**



Aspartate Transcarbamoylase

RCSB PDB | Deposit | Search | Visualize | Analyze | Download | Learn | More | MyPDB Login

RCSB PDB PROTEIN DATA BANK

135201 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands

Go

Advanced Search | Browse by Annotations

PDB-101 | Worldwide PDB | EMDataBank | NDB Nucleic Acid Database | Worldwide Protein Data Bank Foundation

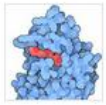
- Welcome
- Deposit
- Search
- Visualize
- Analyze
- Download
- Learn

RCSB PDB-101

Molecular explorations through biology and medicine

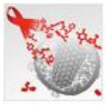
PDB-101 is an online portal for teachers, students, and the general public to promote exploration in the world of proteins and nucleic acids.

Browse all PDB-101 resources by biological theme or start exploring:



Molecule of the Month

Presents short accounts on selected molecules from the Protein Data Bank.

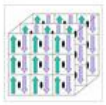


News and Events

Upcoming meetings and events RCSB will hold

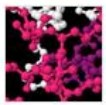
Educational Resources

Access materials that promote exploration in the world of proteins and nucleic acids.



Guide to PDB Data

Understanding PDB Data is a reference to help explore and interpret individual PDB entries.

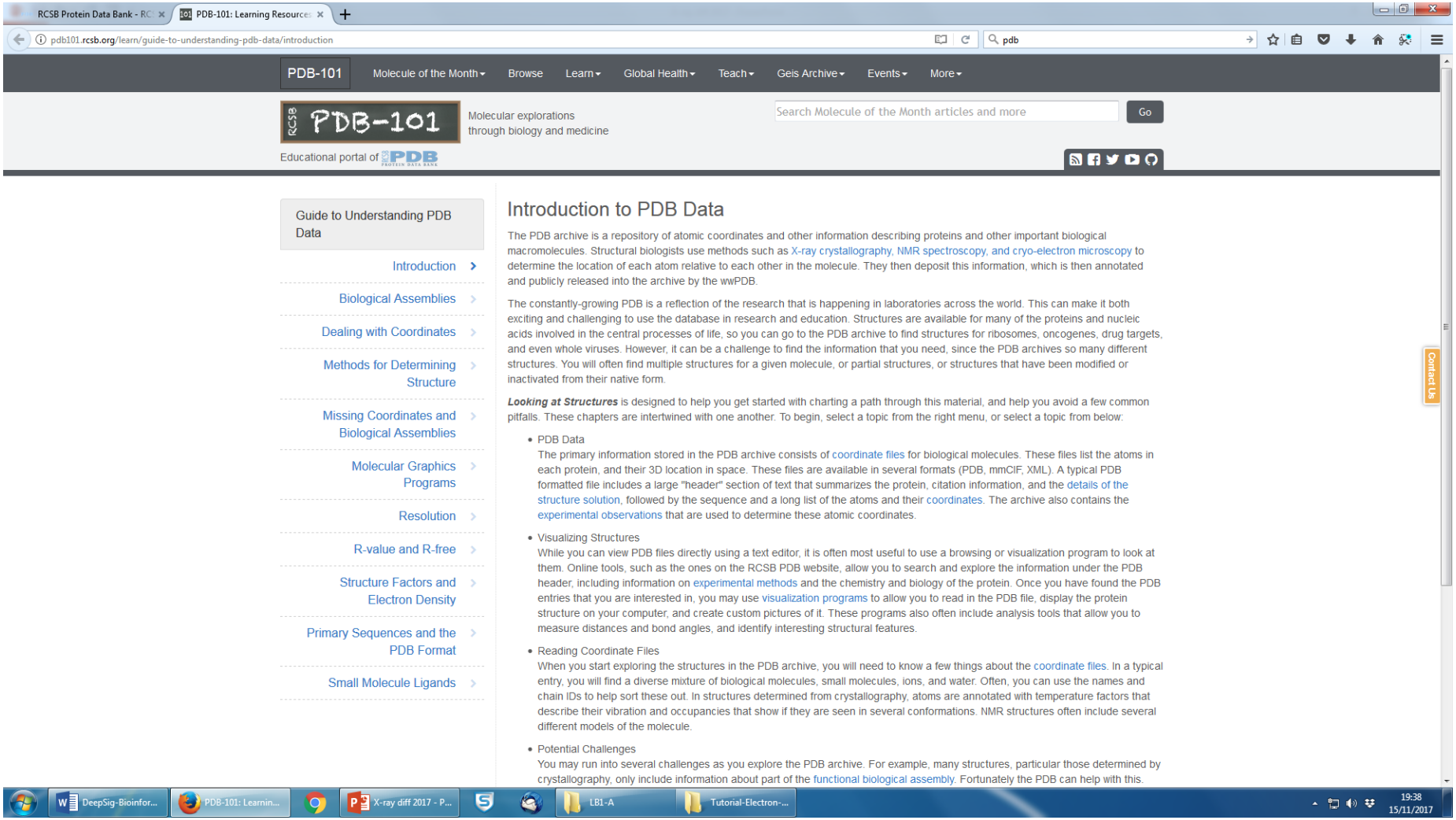


Curricula

Authentic, hands-on teaching materials, individual and group activities.

Geis Digital Archive

View iconic illustrations by the gifted artist Irving Geis (1908-1997) in context with PDB structures and educational information.

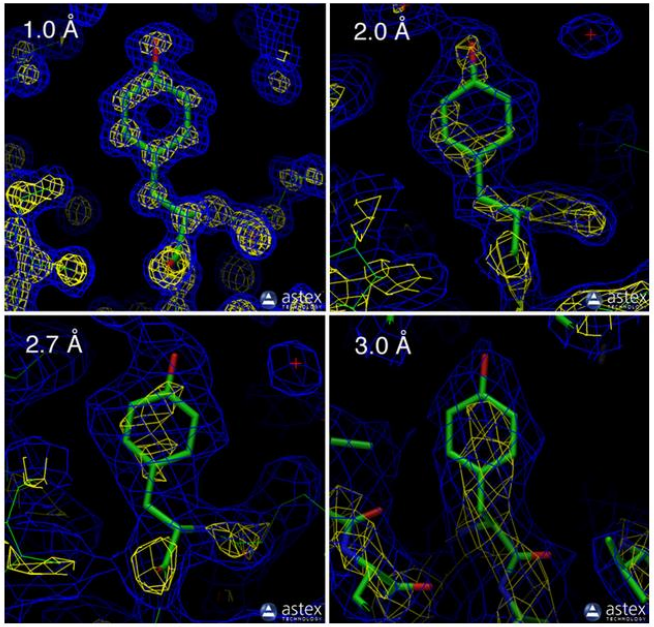

RCSB Protein Data Bank - RC
PDB-101: Learning Resources
pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/introduction
pdb
PDB-101
Molecule of the Month
Browse
Learn
Global Health
Teach
Geis Archive
Events
More
RCSB PDB-101
Molecular explorations through biology and medicine
Educational portal of PDB
Search Molecule of the Month articles and more
Go
Guide to Understanding PDB Data
Introduction
Biological Assemblies
Dealing with Coordinates
Methods for Determining Structure
Missing Coordinates and Biological Assemblies
Molecular Graphics Programs
Resolution
R-value and R-free
Structure Factors and Electron Density
Primary Sequences and the PDB Format
Small Molecule Ligands
Introduction to PDB Data
The PDB archive is a repository of atomic coordinates and other information describing proteins and other important biological macromolecules. Structural biologists use methods such as X-ray crystallography, NMR spectroscopy, and cryo-electron microscopy to determine the location of each atom relative to each other in the molecule. They then deposit this information, which is then annotated and publicly released into the archive by the wwPDB.
The constantly-growing PDB is a reflection of the research that is happening in laboratories across the world. This can make it both exciting and challenging to use the database in research and education. Structures are available for many of the proteins and nucleic acids involved in the central processes of life, so you can go to the PDB archive to find structures for ribosomes, oncogenes, drug targets, and even whole viruses. However, it can be a challenge to find the information that you need, since the PDB archives so many different structures. You will often find multiple structures for a given molecule, or partial structures, or structures that have been modified or inactivated from their native form.
Looking at Structures is designed to help you get started with charting a path through this material, and help you avoid a few common pitfalls. These chapters are intertwined with one another. To begin, select a topic from the right menu, or select a topic from below:
PDB Data
The primary information stored in the PDB archive consists of coordinate files for biological molecules. These files list the atoms in each protein, and their 3D location in space. These files are available in several formats (PDB, mmCIF, XML). A typical PDB formatted file includes a large "header" section of text that summarizes the protein, citation information, and the details of the structure solution, followed by the sequence and a long list of the atoms and their coordinates. The archive also contains the experimental observations that are used to determine these atomic coordinates.
Visualizing Structures
While you can view PDB files directly using a text editor, it is often most useful to use a browsing or visualization program to look at them. Online tools, such as the ones on the RCSB PDB website, allow you to search and explore the information under the PDB header, including information on experimental methods and the chemistry and biology of the protein. Once you have found the PDB entries that you are interested in, you may use visualization programs to allow you to read in the PDB file, display the protein structure on your computer, and create custom pictures of it. These programs also often include analysis tools that allow you to measure distances and bond angles, and identify interesting structural features.
Reading Coordinate Files
When you start exploring the structures in the PDB archive, you will need to know a few things about the coordinate files. In a typical entry, you will find a diverse mixture of biological molecules, small molecules, ions, and water. Often, you can use the names and chain IDs to help sort these out. In structures determined from crystallography, atoms are annotated with temperature factors that describe their vibration and occupancies that show if they are seen in several conformations. NMR structures often include several different models of the molecule.
Potential Challenges
You may run into several challenges as you explore the PDB archive. For example, many structures, particular those determined by crystallography, only include information about part of the functional biological assembly. Fortunately the PDB can help with this.
Contact Us
DeepSig-Bioinfor...
PDB-101: Learnin...
X-ray diff 2017 - P...
LB1-A
Tutorial-Electron-...
19:38
15/11/2017

Guide to Understanding PDB Data

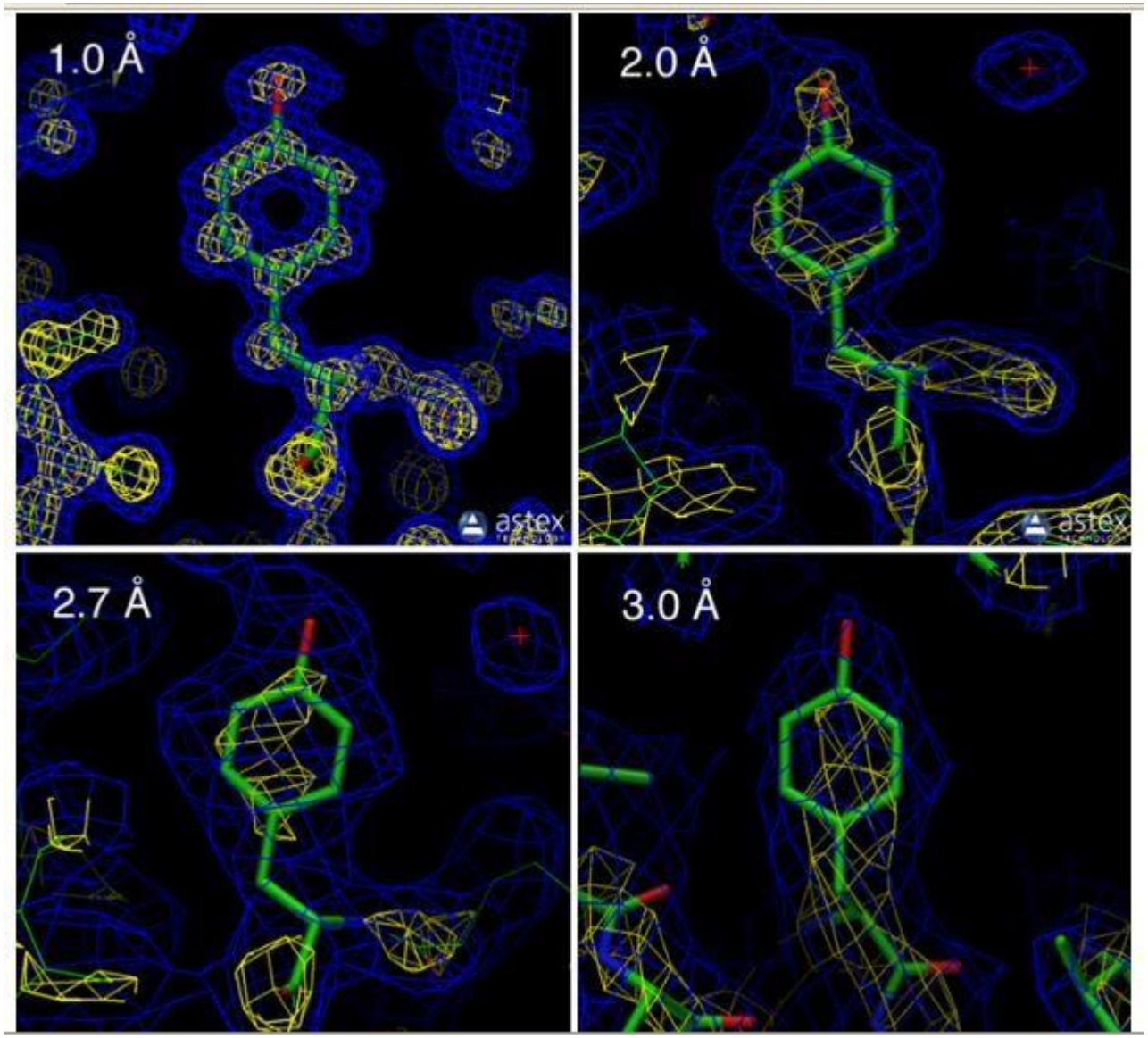
Introduction
Biological Assemblies
Dealing with Coordinates
Methods for Determining Structure
Missing Coordinates and Biological Assemblies
Molecular Graphics Programs
Resolution
R-value and R-free
Structure Factors and Electron Density
Primary Sequences and the PDB Format
Small Molecule Ligands

Resolution

Resolution is a measure of the quality of the data that has been collected on the crystal containing the protein or nucleic acid. If all of the proteins in the crystal are aligned in an identical way, forming a very perfect crystal, then all of the proteins will scatter X-rays the same way, and the diffraction pattern will show the fine details of crystal. On the other hand, if the proteins in the crystal are all slightly different, due to local flexibility or motion, the diffraction pattern will not contain as much fine information. So resolution is a measure of the level of detail present in the diffraction pattern and the level of detail that will be seen when the electron density map is calculated. High-resolution structures, with resolution values of 1 Å or so, are highly ordered and it is easy to see every atom in the electron density map. Lower resolution structures, with resolution of 3 Å or higher, show only the basic contours of the protein chain, and the atomic structure must be inferred. Most crystallographic-defined structures of proteins fall in between these two extremes. As a general rule of thumb, we have more confidence in the location of atoms in structures with resolution values that are small, called "high-resolution structures".



Electron density maps for structures with a range of resolutions are shown. The first three show tyrosine 103 from myoglobin, from entries 1a6m (1.0 Å resolution), 106m (2.0 Å resolution), and 108m (2.7 Å resolution). The final example shows tyrosine 130 from hemoglobin (chain B), from entry 1s0h (3.0 Å resolution). In the pictures, the blue and yellow contours surround regions of high



RESOLUTION

Guide to Understanding PDB Data

- Introduction
- Biological Assemblies
- Dealing with Coordinates
- Methods for Determining Structure
- Missing Coordinates and Biological Assemblies
- Molecular Graphics Programs
- Resolution
- R-value and R-free
- Structure Factors and Electron Density
- Primary Sequences and the PDB Format
- Small Molecule Ligands

R-value and R-free

R-value is the measure of the quality of the atomic model obtained from the crystallographic data. When solving the structure of a protein, the researcher first builds an atomic model and then calculates a simulated diffraction pattern based on that model. The R-value measures how well the simulated diffraction pattern matches the experimentally-observed diffraction pattern. A totally random set of atoms will give an R-value of about 0.63, whereas a perfect fit would have a value of 0. Typical values are about 0.20.

A fit may not be perfect for many reasons. One major reason is that protein and nucleic acid crystals contain large channels of water. The water does not have a defined structure and is not included in the atomic model. Other reasons include disorder and vibration that is not accounted for in the model.

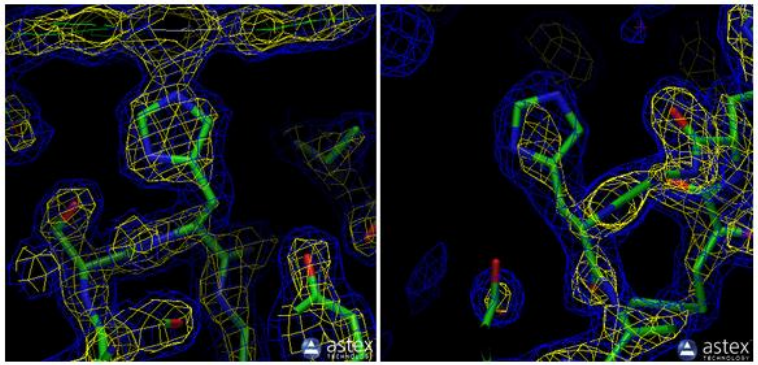
There is one potential problem with using R-values to assess the quality of a structure. The refinement process is often used to improve the atomic model of a given structure to make it fit better to the experimental data and improve the R-value. Unfortunately, this introduces bias into the process, since the atomic model is used along with the diffraction pattern to calculate the electron density. The use of the R-free value is a less biased way to look at this. Before refinement begins, about 10% of the experimental observations are removed from the data set. Then, refinement is performed using the remaining 90%. The R-free value is then calculated by seeing how well the model predicts the 10% that were not used in refinement. For an ideal model that is not over-interpreting the data, the R-free will be similar to the R-value. Typically, it is a little higher, with a value of about 0.26.

For more information on bias and R-values, see "Model Building and Refinement Practice" by G. J. Kleywegt and T. A. Jones, Methods in Enzymology 277, 208-230 (1997).

Temperature Factors

If we were able to hold an atom rigidly fixed in one place, we could observe its distribution of electrons in an ideal situation. The image would be dense towards the center with the density falling off further from the nucleus. When you look at experimental electron density distributions, however, the electrons usually have a wider distribution than this ideal. This may be due to vibration of the atoms, or differences between the many different molecules in the crystal lattice. The observed electron density will include an average of all these small motions, yielding a slightly smeared image of the molecule.

These motions, and the resultant smearing of the electron density, are incorporated into the atomic model by a B-value or temperature factor. The amount of smearing is proportional to the magnitude of the B-value. Values under 10 create a model of the atom that is very sharp, indicating that the atom is not moving much and is in the same position in all of the molecules in the crystal. Values greater than 50 or so indicate that the atom is moving so much that it can barely been seen. This is often the case for atoms at the surface of proteins, where long sidechains are free to wag in the surrounding water.



The example shown is from a myoglobin structure solved at a 2.0 Å resolution (PDB entry 1mbi). Two histidine amino acids are shown. On the left is HIS93, which coordinates with the iron atom and thus, is held firmly in place. It has B-values in the range of 15-20 -- notice how the contours nicely surround the whole amino acid, revealing a sharp electron density. On the right is HIS81, which is exposed on the surface of the protein and has higher B-values in the range of 22-74. Notice how the contours enclose a smaller space, showing a smaller region with high electron density for this amino acid because the overall electron density is weakly smeared in the space around the contours. These pictures are created using the Astex viewer, which is available on the Structure Summary page for this PDB entry (just click the "EDS" link in the "Experimental Method" section).

A data base of protein diffraction maps

pdb

Home | About | Browse | Statistics | Submit data | News | Login

Search diffraction images

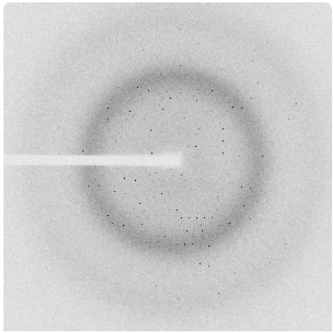
NIH National Institutes of Health
Office of the Director
Data Science at NIH

Integrated Resource for Reproducibility in Macromolecular Crystallography

This project is being funded by the Targeted Software Development award 1 U01 HG008424-01 as part of the BD2K (Big Data to Knowledge) program of the National Institute of Health. The project is developing tools for "wrangling" data from protein diffraction experiments. We are also creating a growing repository of diffraction experiments used to determine protein structures in the PDB, contributed by the CSGID, SSGCID, JCSG, MCSG, SGC, and other large-scale projects, as well as individual research laboratories.

Currently indexed projects: **3376**

Currently indexed datasets: **6365**



https://proteindiffraction.org/

Browse & search | Statistics | Submit data | Publications | Beamlines | Educational resources

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB Login

RCSB PDB PROTEIN DATA BANK 135201 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

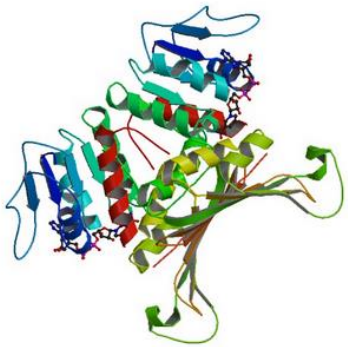
Search by PDB ID, author, macromolecule, sequence, or ligands Go

Advanced Search | Browse by Annotations

PDB-101 wwPDB EMDataBank NDB Nucleic Acid Database Worldwide Protein Data Bank Foundation

Structure Summary | 3D View | Annotations | Sequence | Sequence Similarity | Structure Similarity | Experiment

Biological Assembly 1



View in 3D: NGL or JSmol (in Browser)

Standalone Viewers

Simple Viewer Protein Workshop
Ligand Explorer Kiosk Viewer

Protein Symmetry: Cyclic - C2 (View in 3D)

Protein Stoichiometry: Homo 2-mer - A2

Biological assembly 1 assigned by authors and generated by PISA,PQS (software)

Display Files Download Files

1J5P

Crystal structure of aspartate dehydrogenase (TM1643) from Thermotoga maritima at 1.9 A resolution

DOI: 10.2210/pdb1j5p/pdb

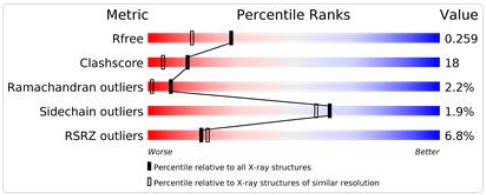
PSI Protein Structure Initiative

Classification: OXIDOREDUCTASE
Deposited: 2002-06-27 Released: 2002-07-10
Deposition author(s): Joint Center for Structural Genomics
Organism: Thermotoga maritima
Expression System: Escherichia coli

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.9 Å
R-Value Free: 0.260
R-Value Work: 0.224

wwPDB Validation 3D Report Full Report



Literature Download Primary Citation

Crystal structure of aspartate dehydrogenase (TM1643) from Thermotoga maritima at 1.9 A resolution

Joint Center for Structural Genomics

http://www.rcsb.org/pdb/explore.do?structureId=1j5p