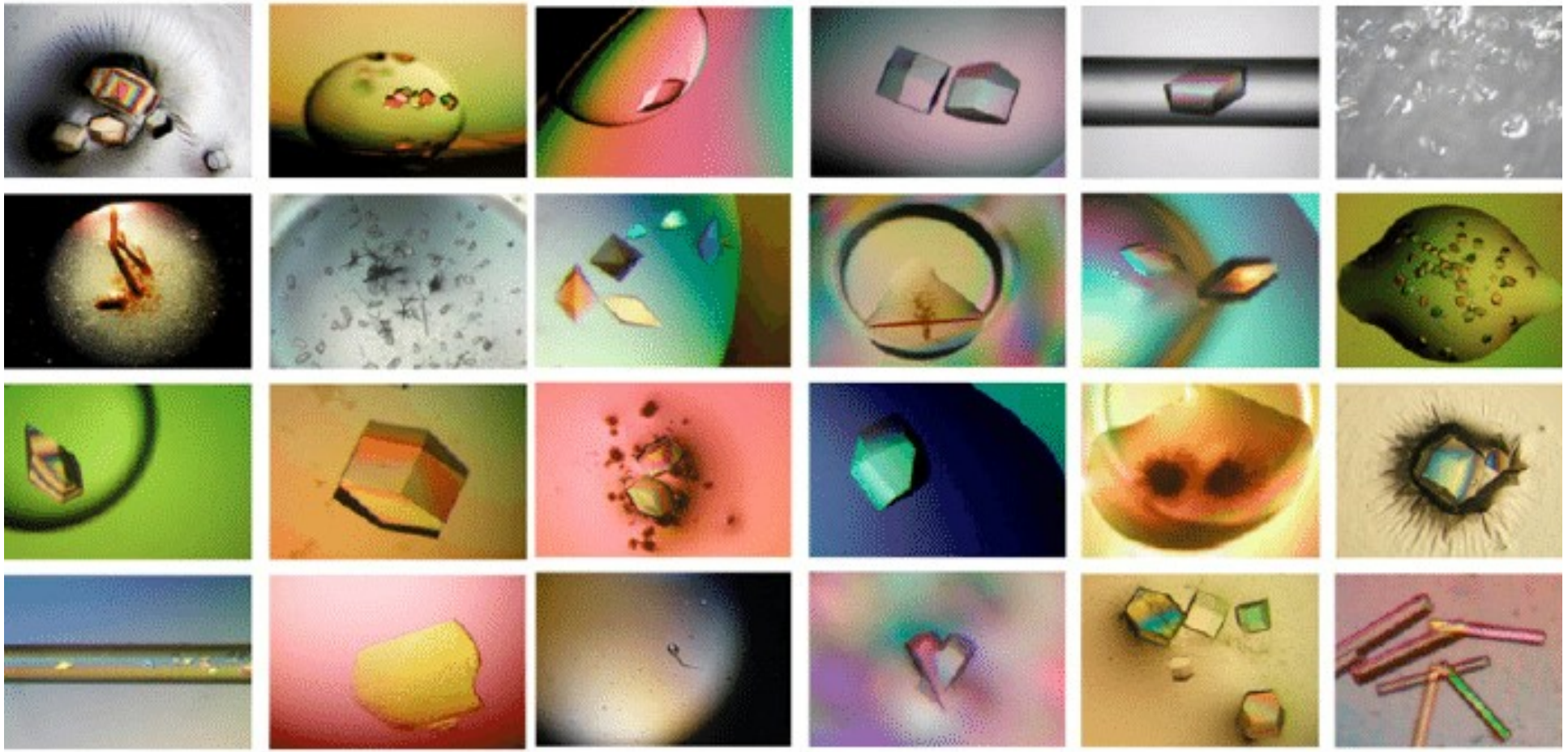
Crystal geometry

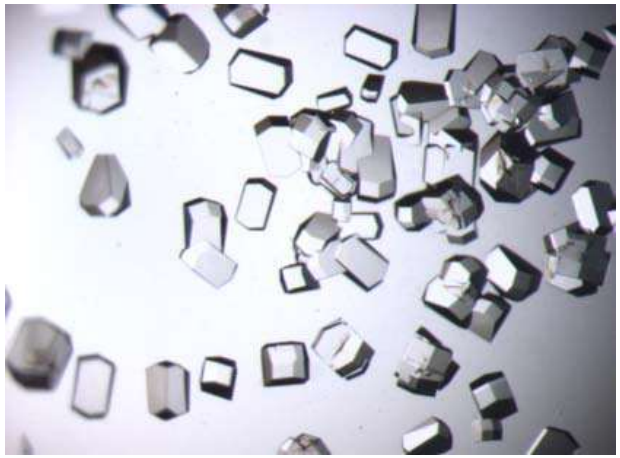


Biocrystallography and Electron Microscopy rdezorzi@units.it

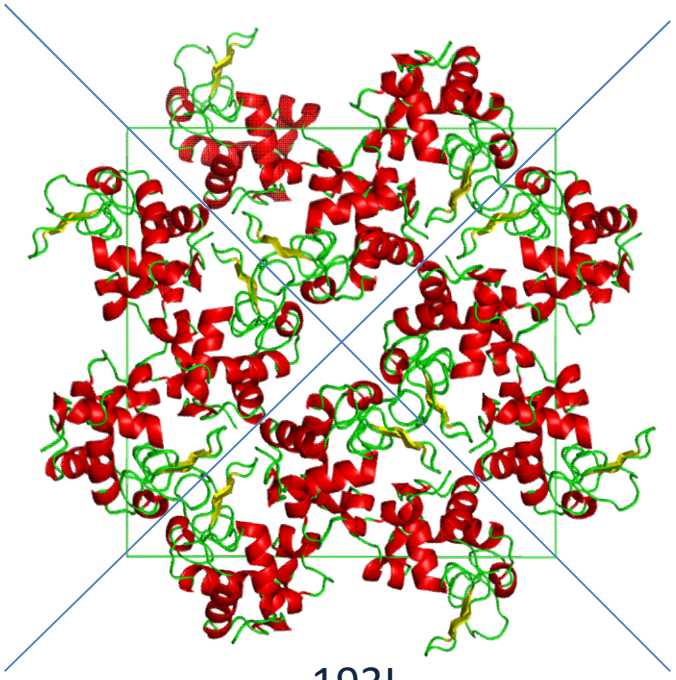
Sharp edges and plane faces

Regular crystal habit depends on the internal long-range order of the crystal structure.

Diffraction properties of crystals depend on their internal order: X-ray interaction with the ordered molecules forming the crystal.



Combination of the requirements for:
long-range order
and
symmetry elements in the crystal
=
230 **space groups** for crystals,
But only **65** allowed for protein crystals



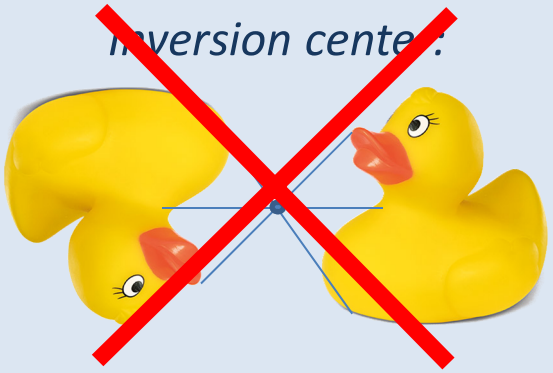
193L

Understanding crystal order is important to maximize the information that can be extracted from crystallographic data.

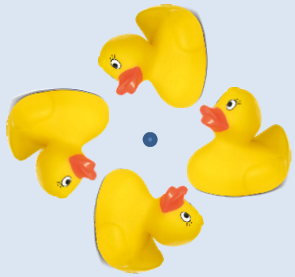
Point group symmetry elements

Point group symmetry elements are invariant points of transformations able to relate a point (x,y,z) to another point (x',y',z').

Inversion center:



Rotation axis:



Mirror plane:

During each of this transformations, a generic point of coordinates (x,y,z) is transformed in a symmetric point, with coordinates (x',y',z'), by a matrix operator:

Inversion center, i:

$$\boldsymbol{x'} = i\,\boldsymbol{x}$$

$$i = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

Rotation axis, e.g. 4 along z:

$$\boldsymbol{x'} = A\,\boldsymbol{x}$$

$$A = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Mirror plane, e.g. in yz:

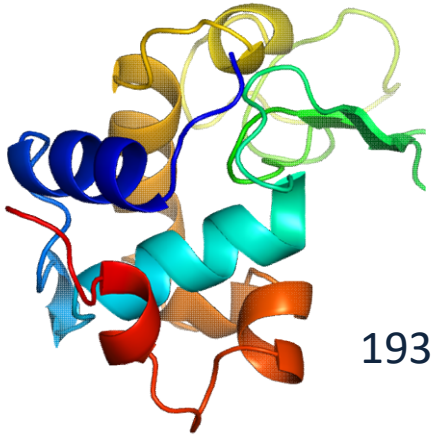
$$\boldsymbol{x'} = m\,\boldsymbol{x}$$

$$m = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation axes

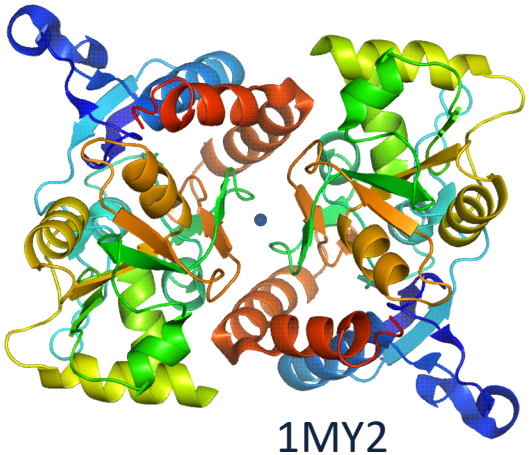
A rotation operation *n* (or of order *n*) describes a rotation of each point of *360°/n* around the rotation axis:

1 Rotation of 360° (identity!)



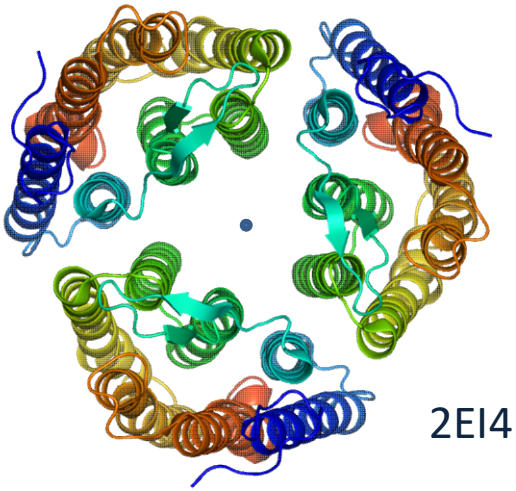
193L

2 Rotation of 180°



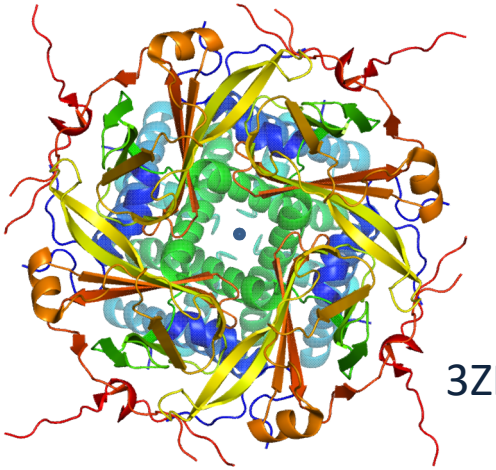
1MY2

3 Rotation of 120°



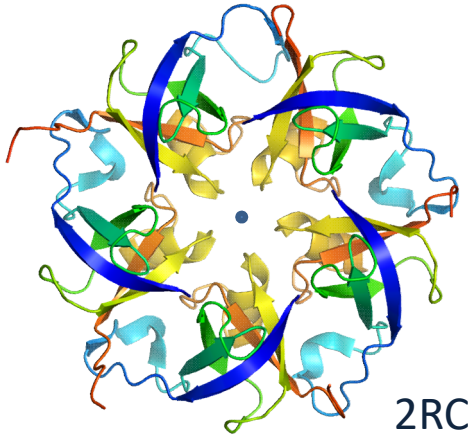
2EI4

4 Rotation of 90°



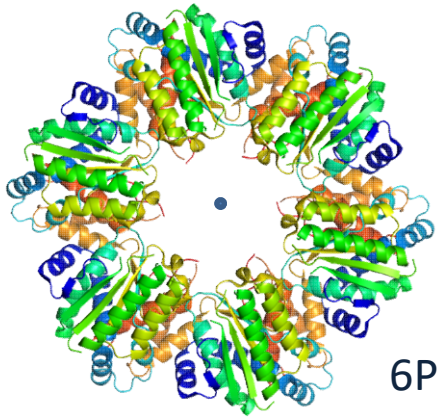
3ZRS

5 Rotation of 72°



2RCF

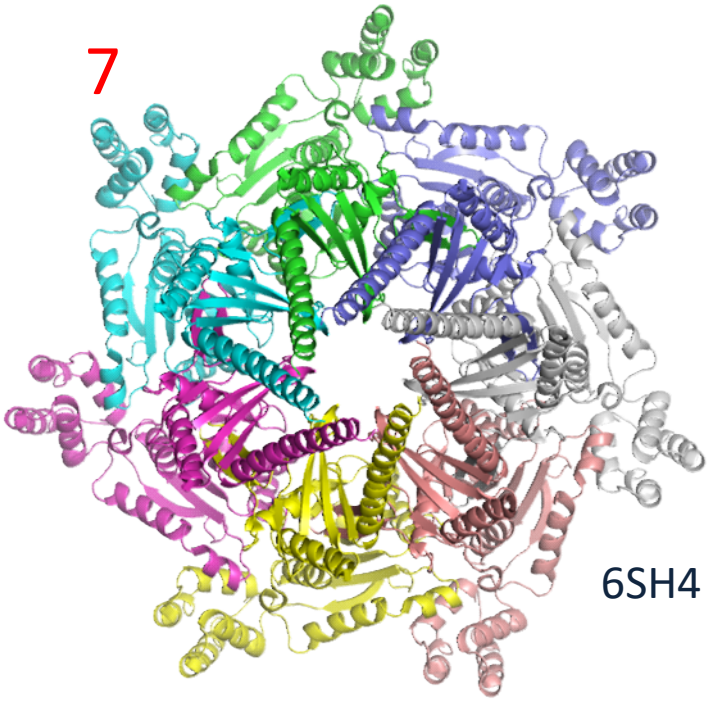
6 Rotation of 60°



6PB3

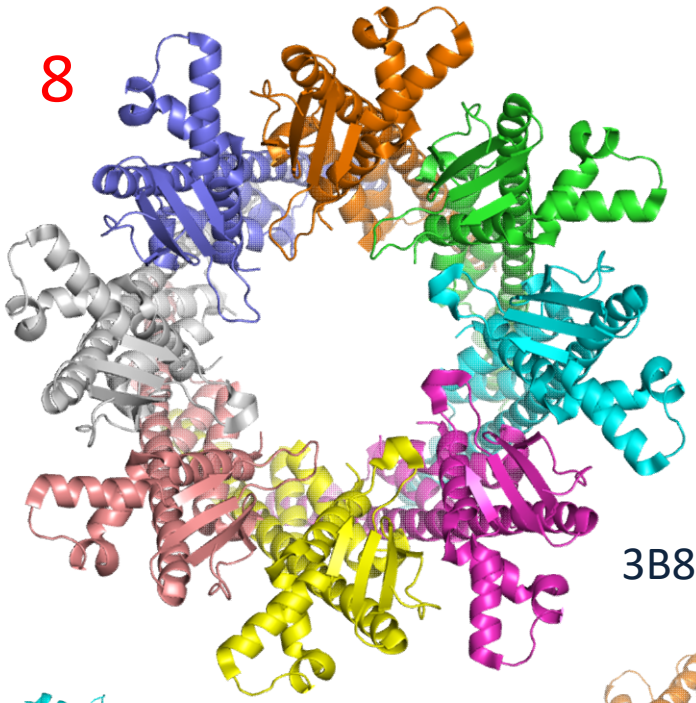
And more:

7



6SH4

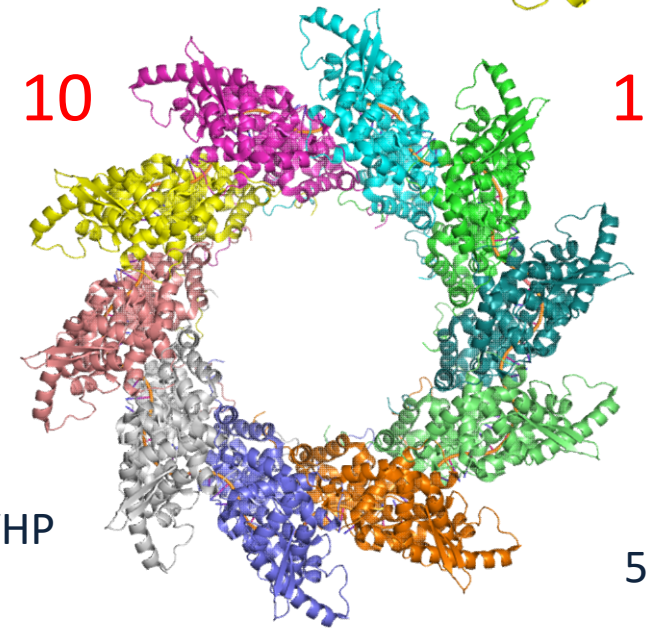
8



3B8O

When symmetry elements are present, they involve more than one protein chain: proteins are ASYMMETRIC!

10



2YHP

12

5NBZ

Translational periodicity: lattice and unit cell

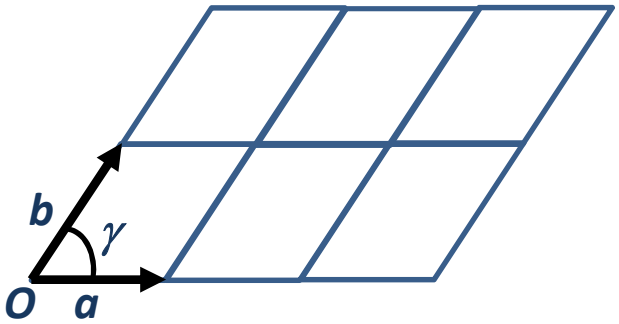
Crystals are formed by repeated units along the three directions, but to simplify the problem we can start to describe lattice in the 2D case

How to cover a floor with tiles??

Due to the requirement for **translational periodicity**, lattices can have only the following rotational symmetries:

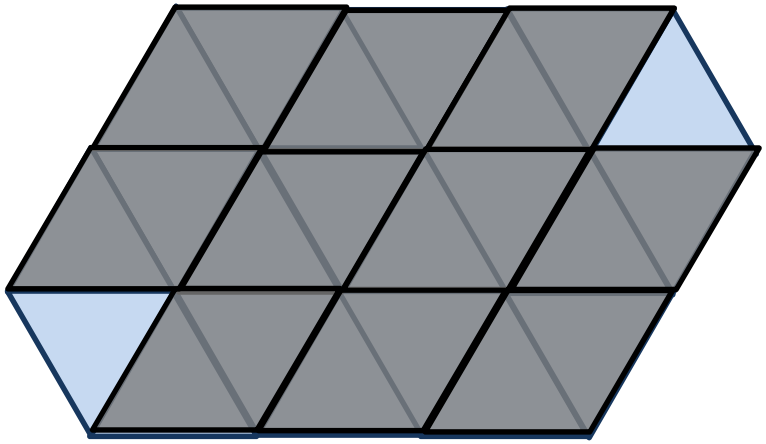
1, **2**, **3**, **4** and **6**

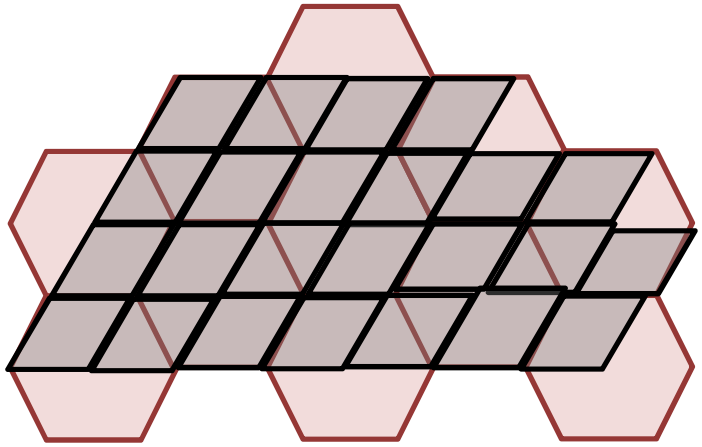
In 2D, the lattice is formed by a repeted unit, translated in 2 directions:



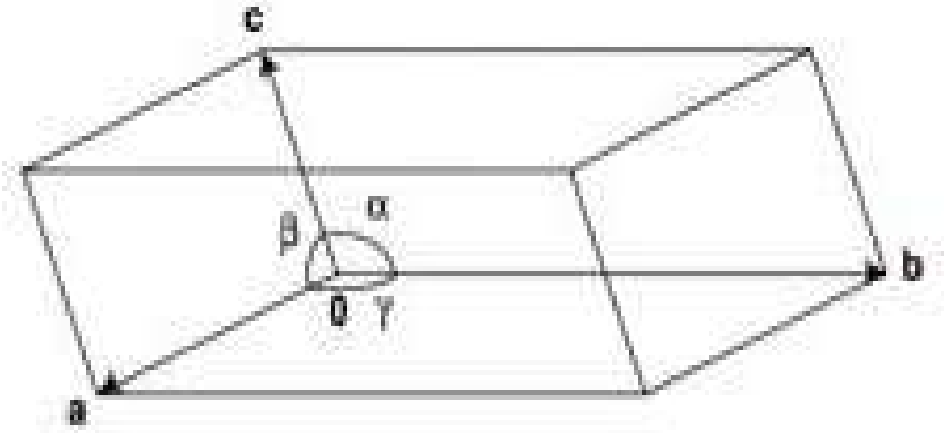
The repetitive unit is called **unit cell**. The lattice is defined by an **origin** of the translations and the **unit cell parameters** (or dimensions): (in 2D) a, b and γ

Even when symmetry elements include a 3-fold axis or a 6-fold axis, unit cell can be described as a parallelogram:





In 3D:



Unit cell parameters:
a, *b*, *c* and α, β, γ

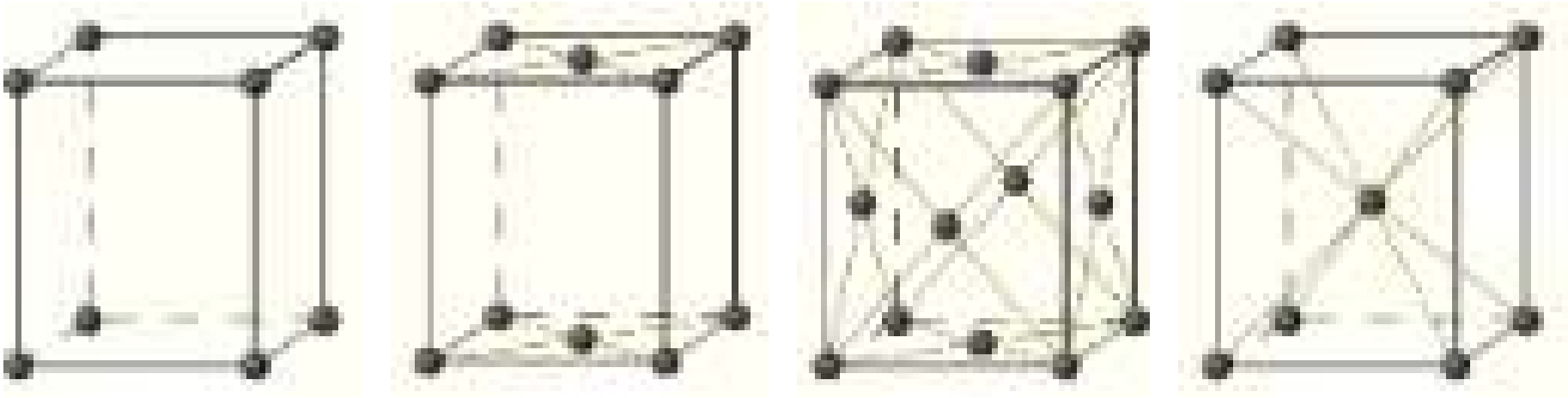
Crystal families and crystal systems

Crystal family	Crystal system	Unit cell dimensions	Minimal symmetry elements
Triclinic	Triclinic	***a***, ***b***, ***c***, α, β, γ	none
Monoclinic	Monoclinic	***a***, ***b***, ***c***, β (α, γ=90°)	2
Orthorhombic	Orthorhombic	***a***, ***b***, ***c*** (α=β=γ=90°)	three perpendicular 2 axes
Tetragonal	Tetragonal	***a***, ***c*** (*b*=*a*, α=β=γ=90°)	4
Hexagonal	Trigonal	***a***, ***c*** (*b*=*a*, α=β=90°, γ=120°)	3
	Hexagonal		6
Cubic	Cubic	***a*** (*b*=*a*, *c*=*a*, α=β=γ=90°)	four 3 axes along diagonal directions

Primitive and centered lattices

Primitive lattices have *nodal points* (*nodes*) at the vertices of the unit cell.

But further translations are possible in the unit cell, forming **centered lattices**, with additional nodes:



Primitive lattice

Base centered

Face centered

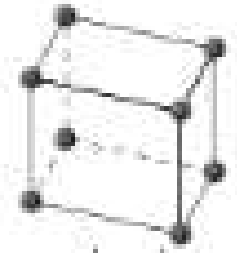
Face(s) centered lattices

Body centered lattice

A primitive lattice can **always** describe the structure, but in presence of specific elements of symmetry it can be useful to describe the lattice as centered.

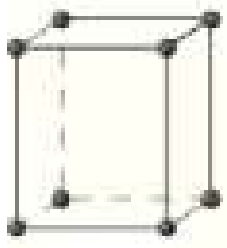
Crystal families + centering = 14 Bravais lattices

Triclinic lattice

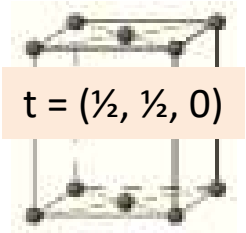


Primitive, P

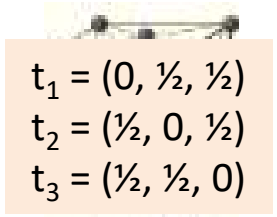
Orthorhombic lattice



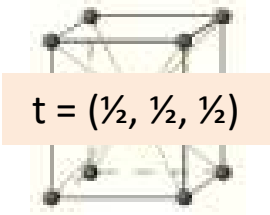
Primitive, P



Base centered, C

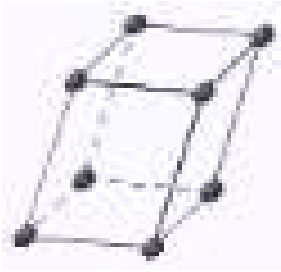


Face centered, F

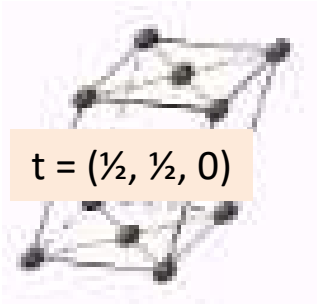


Body centered, I

Monoclinic lattice

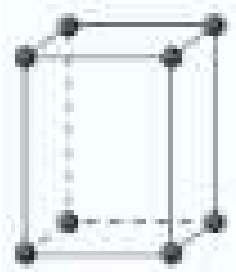


Primitive, P

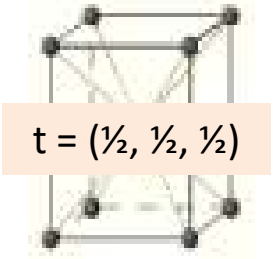


Base centered, C

Tetragonal lattice

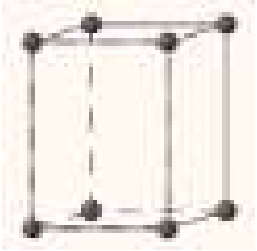


Primitive, P

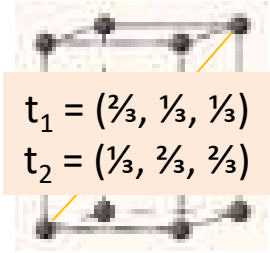


Body centered, I

Hexagonal lattice

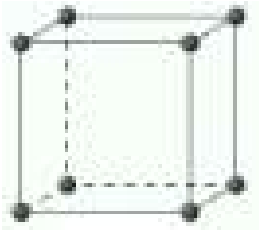


Primitive, P

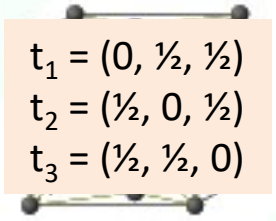


Rhombohedral, R

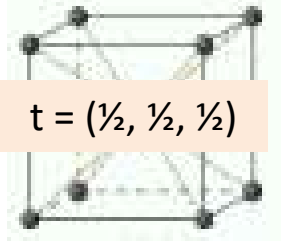
Cubic lattice



Primitive, P



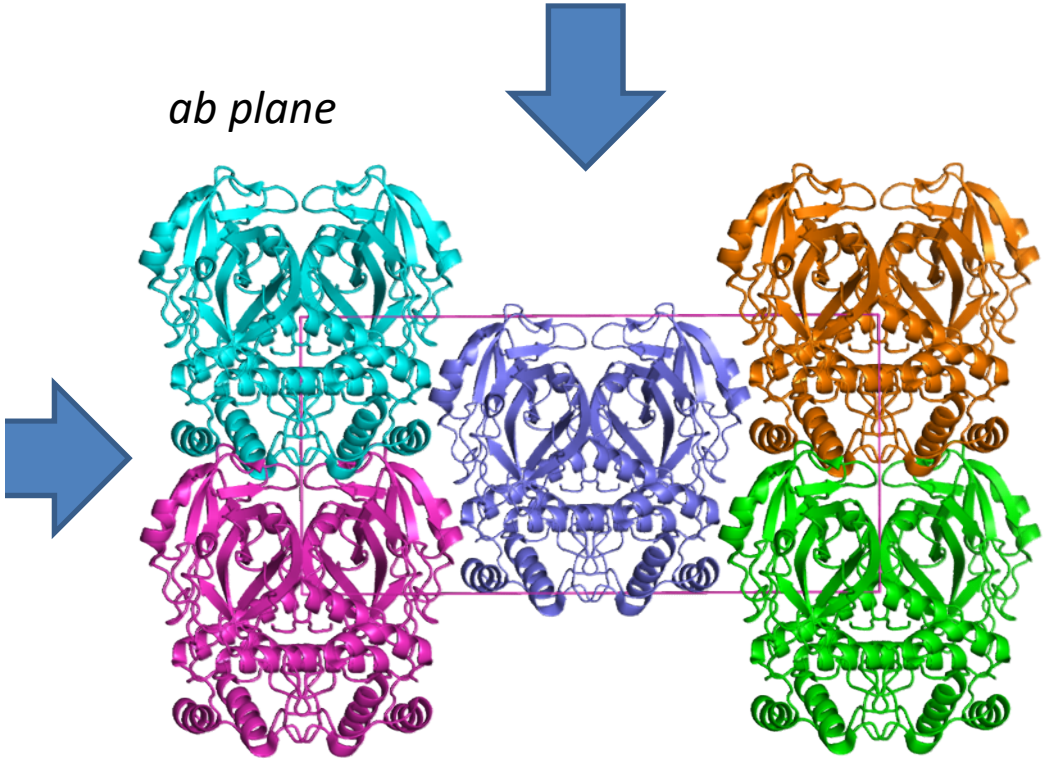
Face centered, F



Body centered, I

Case in point: monoclinic *C2* lattice

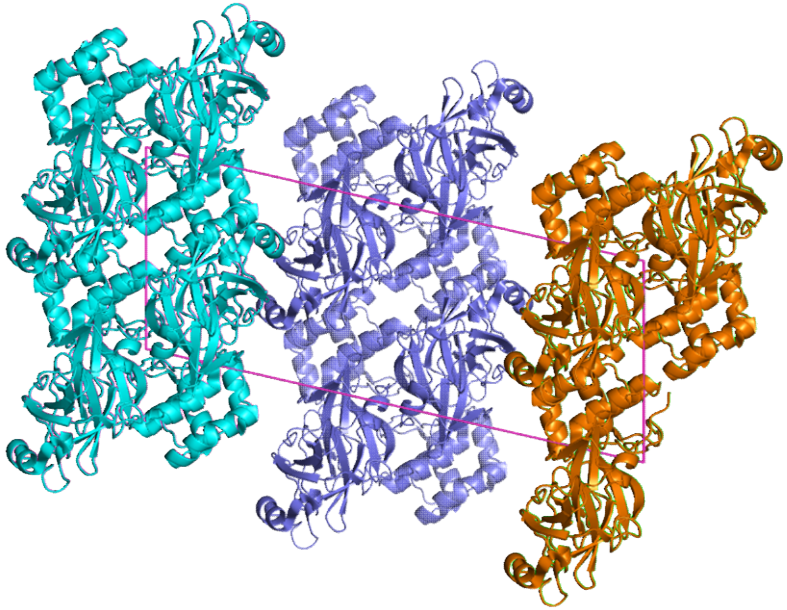
ab plane



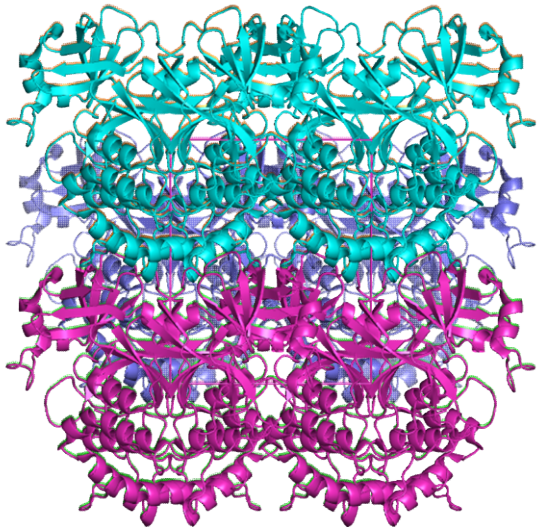
5RE9

Monoclinic:
a, *b*, *c*
$\alpha=\gamma=90°, \beta$

ac plane



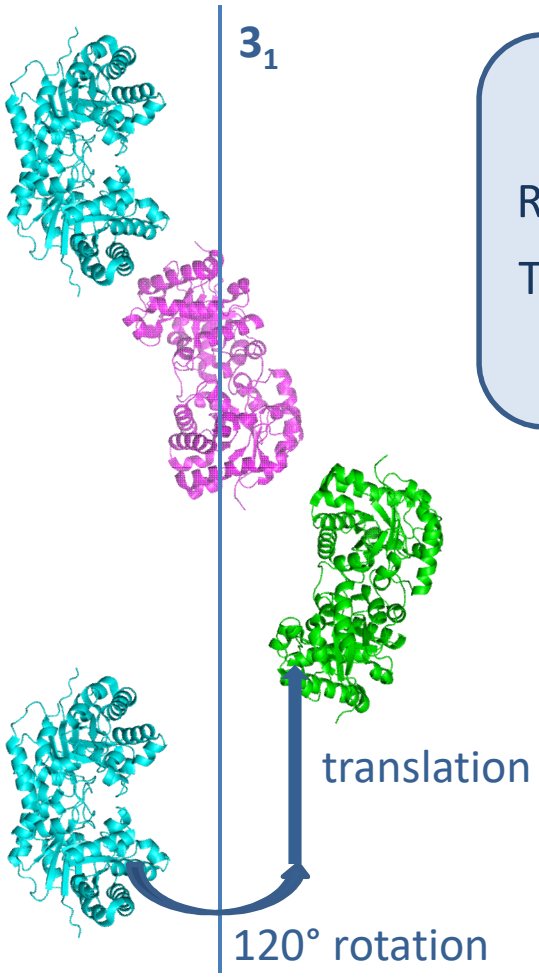
bc plane



Rotation + translation = screw axis

Besides the point group symmetry elements, additional symmetry elements are possible in crystal cells:

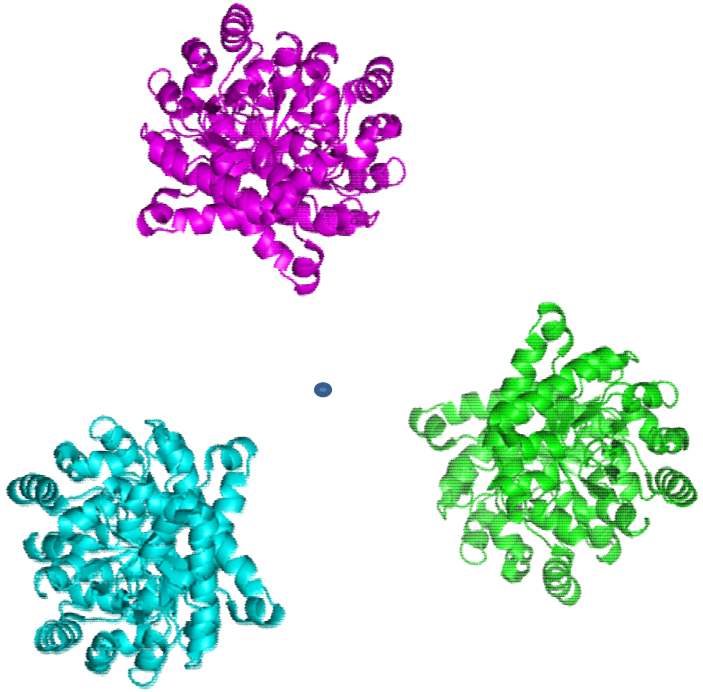
- ***screw axis*** *= rotation + translation*
- *glide planes = mirror + translation*



Screw axis N_m

Rotation of *360°/N*

Translation of *m/N* of the unit cell



Screw axis 3_1

Rotation of *360°/3*

Translation of *1/3* of the unit cell

Rotation + translation = screw axis

Screw axis 3_1

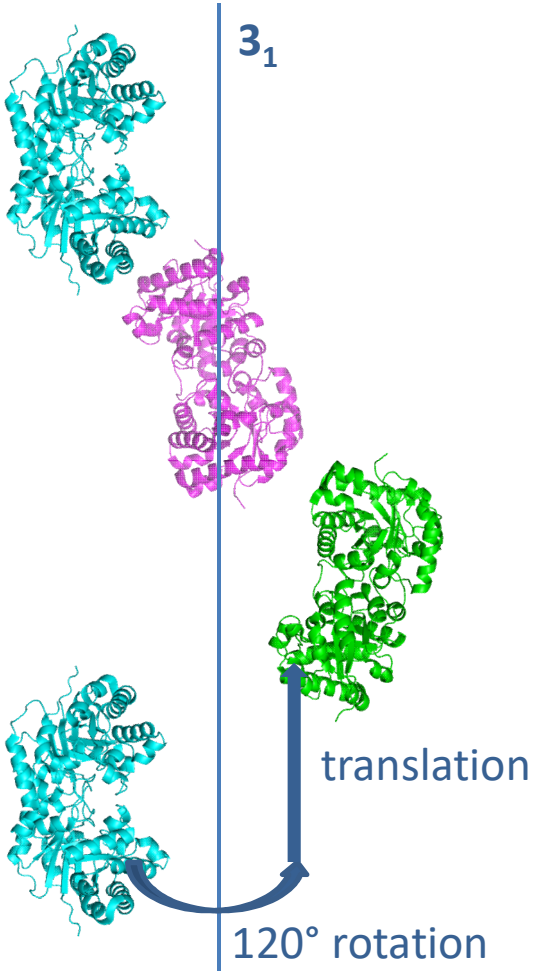
Rotation of *360°/3*

Translation of *1/3* of the unit cell

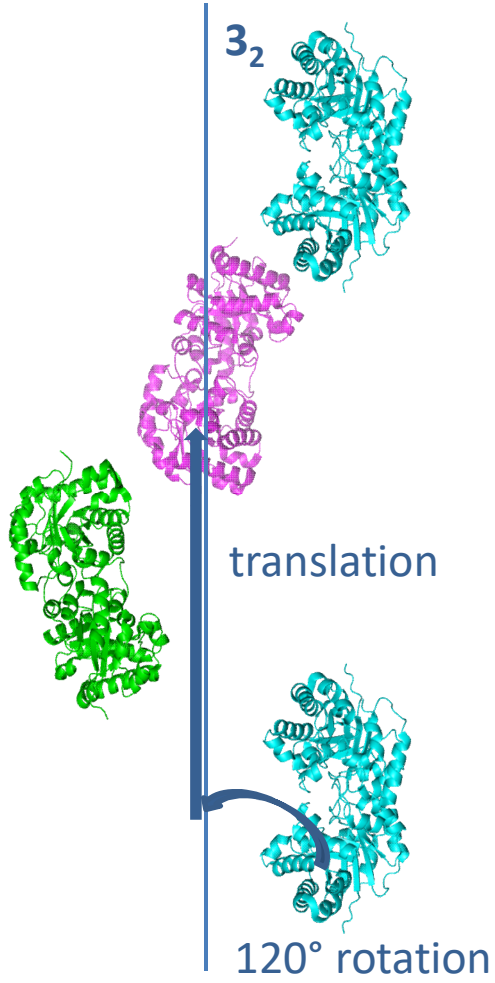
Screw axis 3_2

Rotation of *360°/3*

Translation of *2/3* of the unit cell

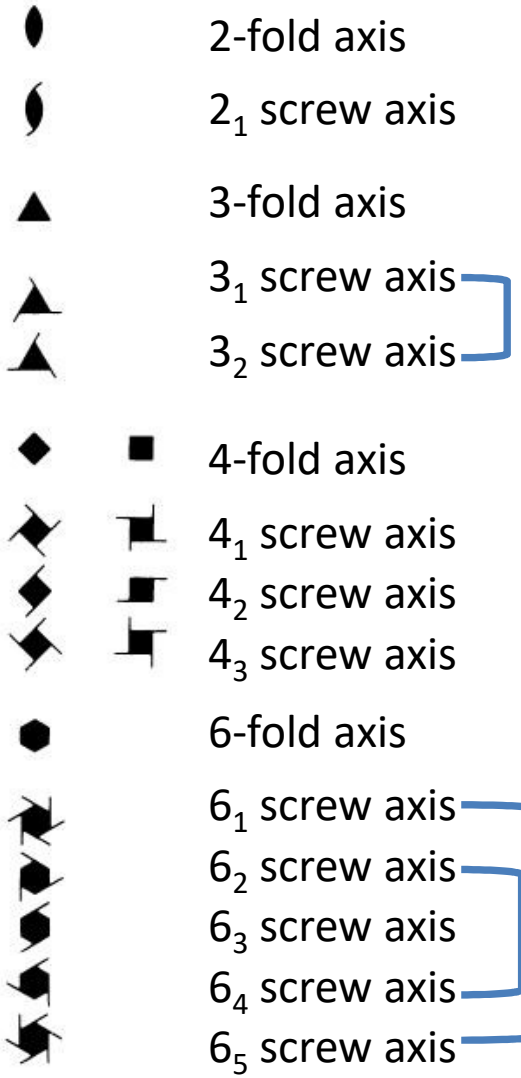


6R8H



Symmetry operations

Symmetry operations are represented with specific figures when perpendicular to the plane, or arrows when parallel to the plane of the figure:



2-fold axis

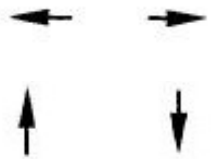
2_1 screw axis

3-fold axis

3_1 screw axis

3_2 screw axis

Rototranslations in opposite directions!



Rotation axes

4-fold axis

4_1 screw axis

4_2 screw axis

4_3 screw axis

6-fold axis

6_1 screw axis

6_2 screw axis

6_3 screw axis

6_4 screw axis

6_5 screw axis

Rototranslations in opposite directions!

Rototranslation axes

Intermolecular contacts and crystal packing

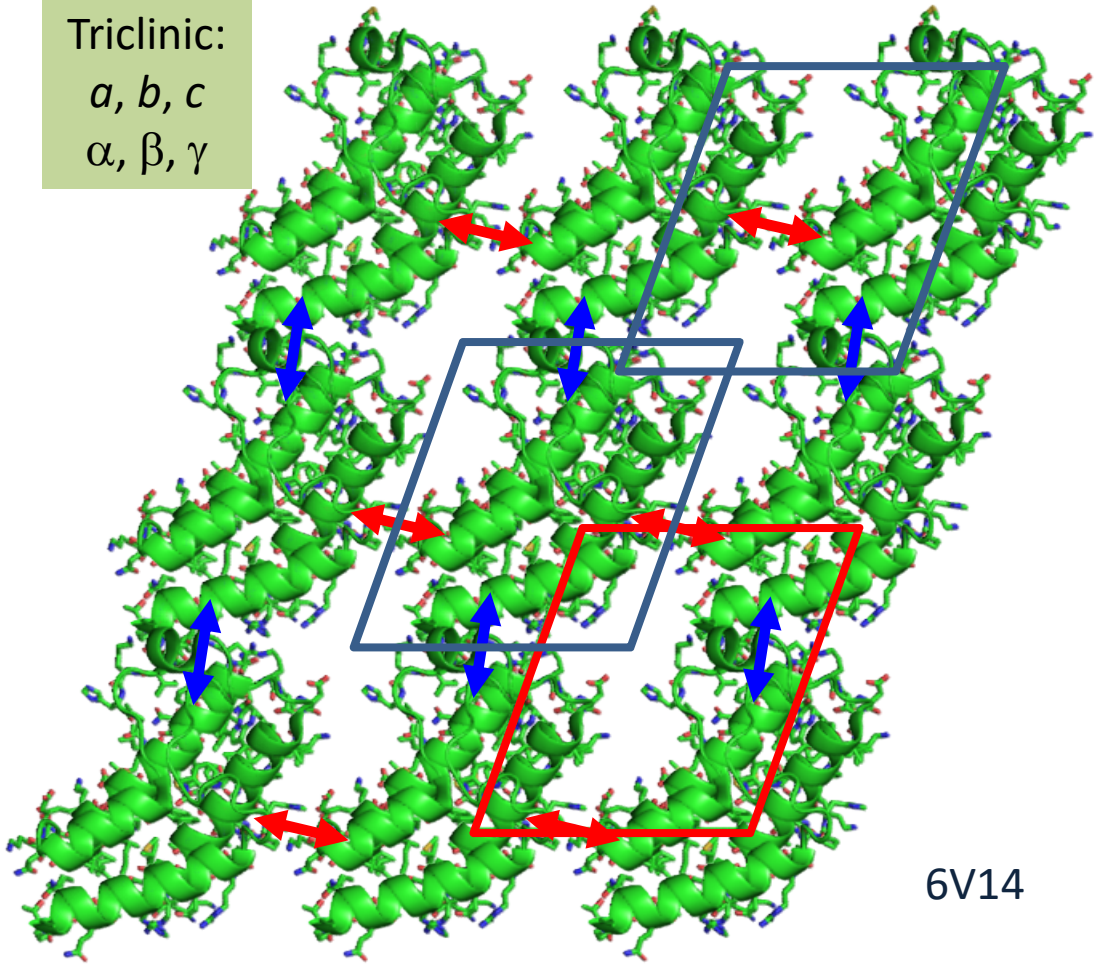
Crystals are held together by intermolecular contacts, that determine their packing:

Crystal packing must be evaluated:

1) to evaluate the effect of crystal contacts on protein conformation

2) to obtain biologically active unit (for symmetry related oligomers)

Triclinic:
a, *b*, *c*
α, β, γ



6V14

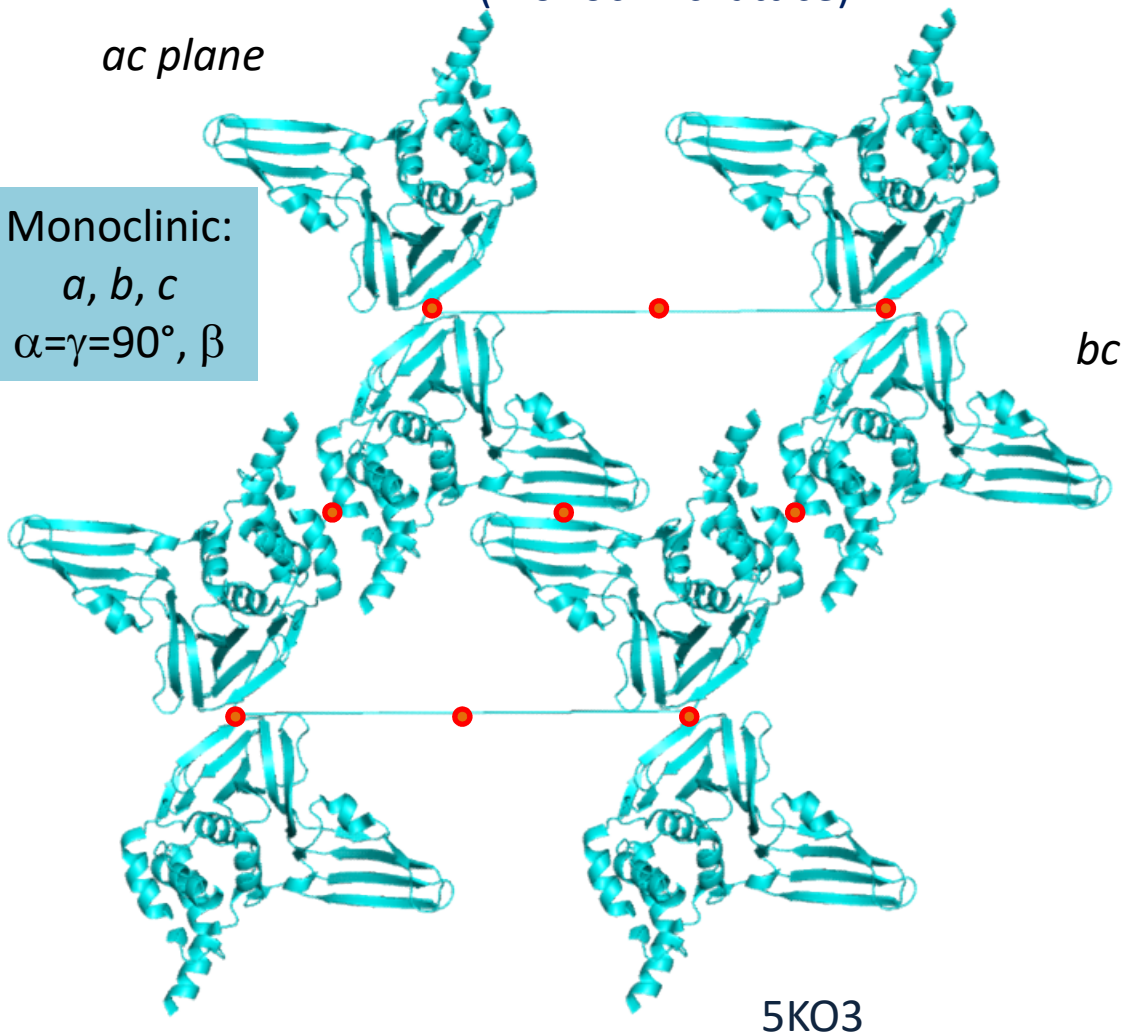
Different **origin** choices are possible (while unit cell dimensions are the same!) for a lattice with no additional symmetry.

Choice of the origin

The choice of the origin depends on the symmetry of the crystal lattice.

Case in point: lattice with 2-fold axis along *b*
(monoclinic lattice)

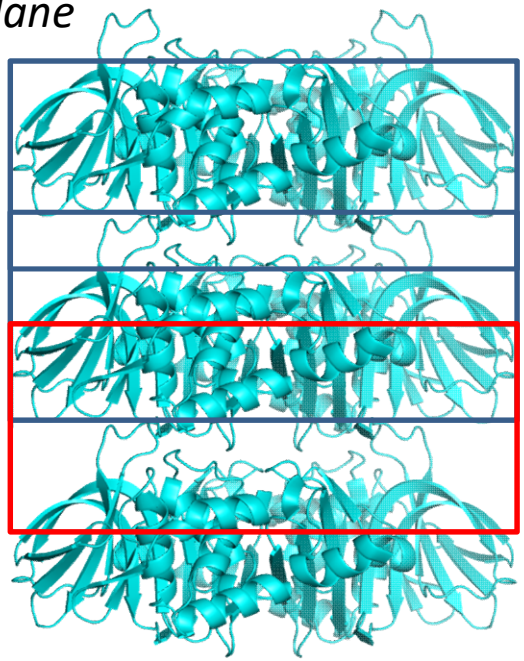
ac plane



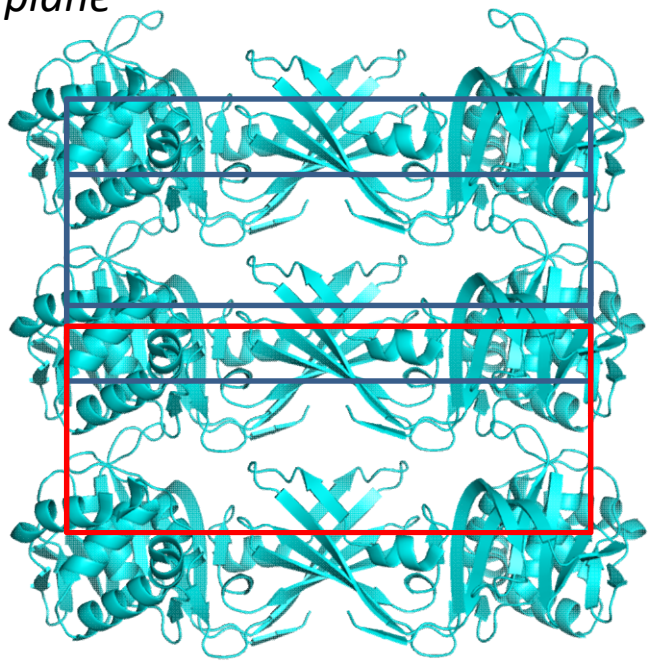
Monoclinic:
a, *b*, *c*
$\alpha=\gamma=90°$, β

5KO3

ab plane



bc plane

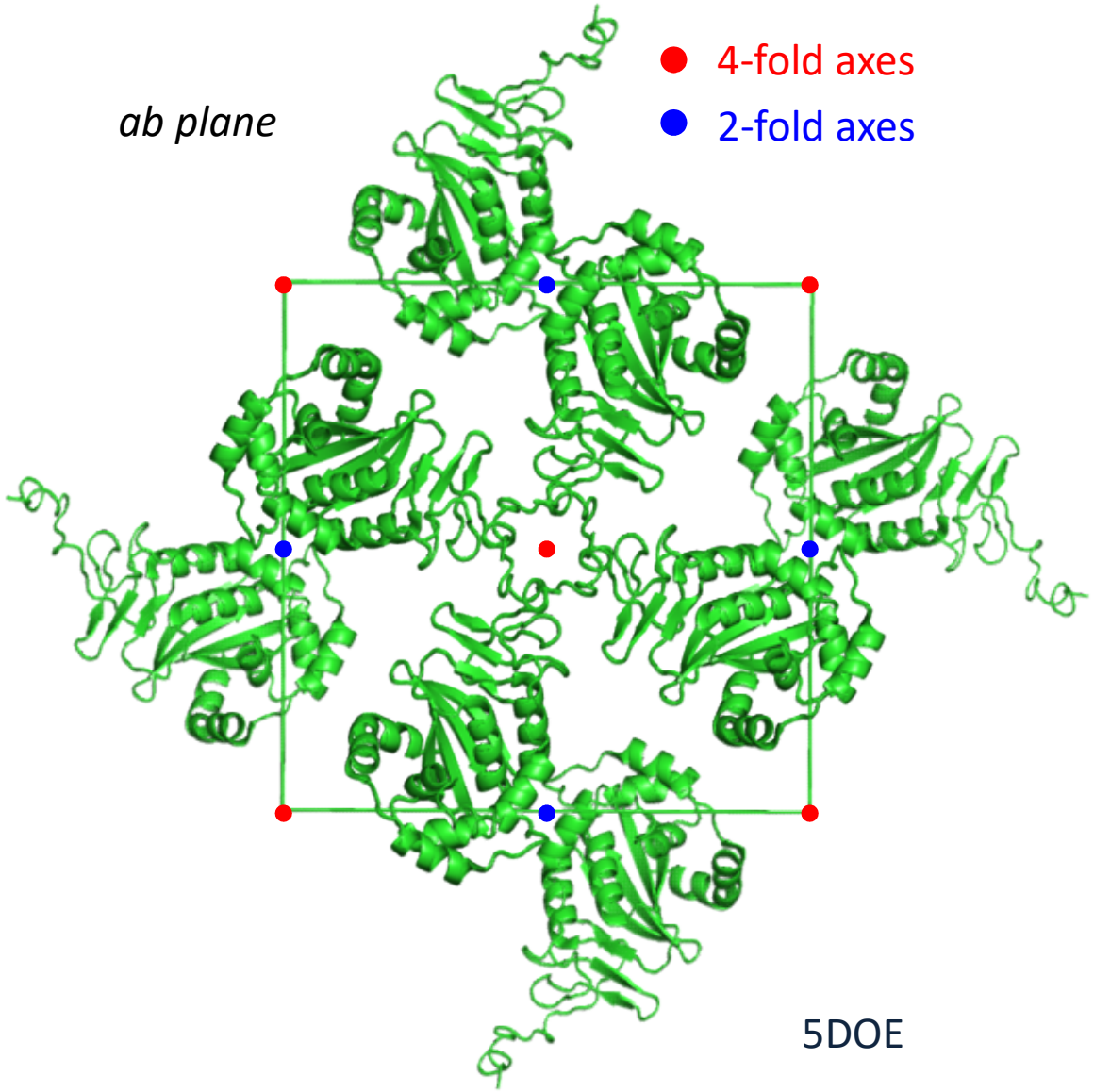


Choice of the origin

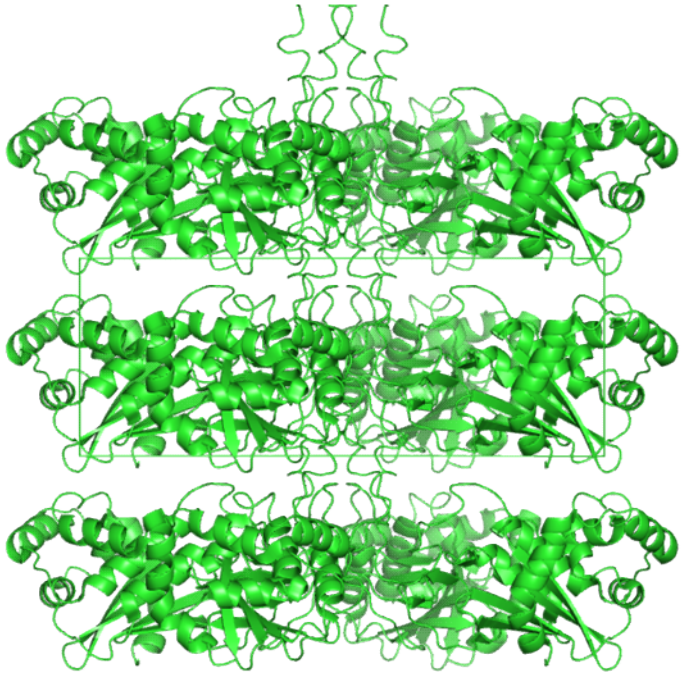
Tetragonal:
a=*b*, *c*
α=β=γ=90°

Case in point: lattice with 4-fold axis along *c* (tetragonal lattice)

ab plane



ac and bc planes



5DOE

Fractional coordinates

Each symmetry operation can be represented by:

(1) a square matrix **S** and (2) a translation vector **t**

that transform a generic point ***x*** with coordinates (*x*,*y*,*z*) in its symmetric ***x'*** with coordinates (x',y',z'): $\boldsymbol{x'} = \boldsymbol{S} \cdot \boldsymbol{x} + \boldsymbol{t}$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} s_{11} & s_{12} & s_{13} \\ s_{21} & s_{22} & s_{23} \\ s_{31} & s_{32} & s_{33} \end{bmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_x \\ t_y \\ t_z \end{pmatrix}$$

The coordinate system of this equation, however, is not the orthogonal system in which we describe the atomic structure with distances in Å (i.e. in the pdb file).

The matrices **S** and vectors **t** are defined in the coordinate system of each specific lattice, i.e. having the *x*,*y*,*z* directions along the translational vectors that define the lattice. In addition, this coordinate system has **fractional coordinates**, that are calculated as fractions of the unit cell parameters in each direction.

Example: the coordinate system of a monoclinic lattice has 2 directions (x and z) that are not perpendicular, but form an angle equal to β.

Transformation: 4-fold axis along *c* direction of a tetragonal lattice

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Transformation: 2_1 screw axis along the *b* direction

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ {}^{1}/_{2} \\ 0 \end{pmatrix}$$