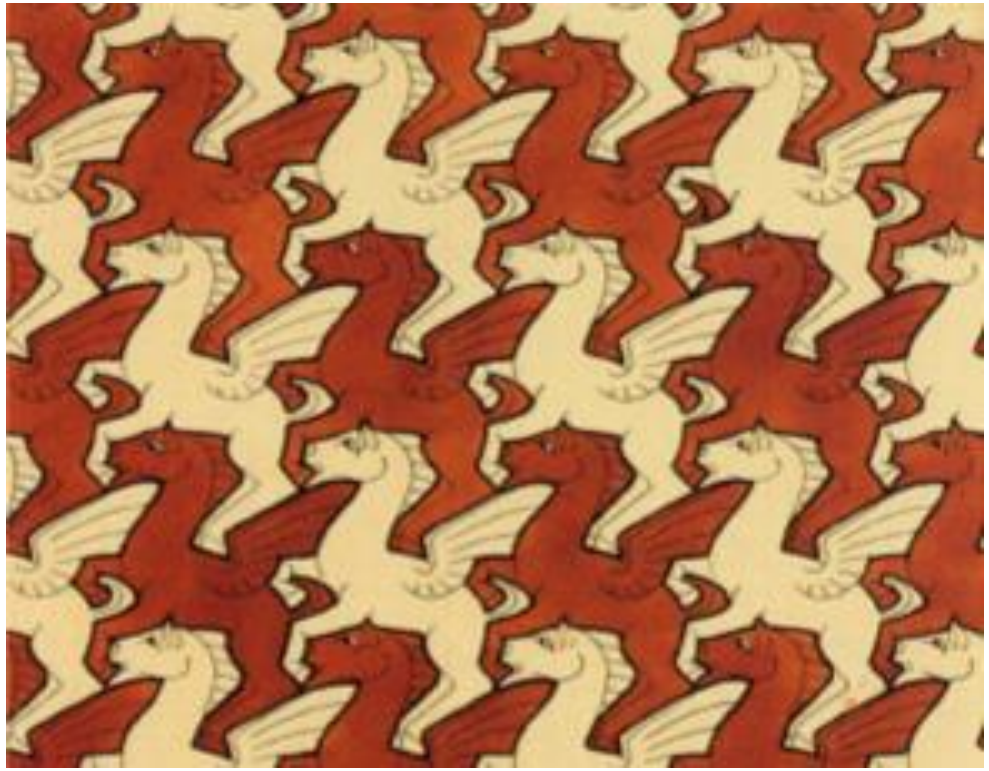
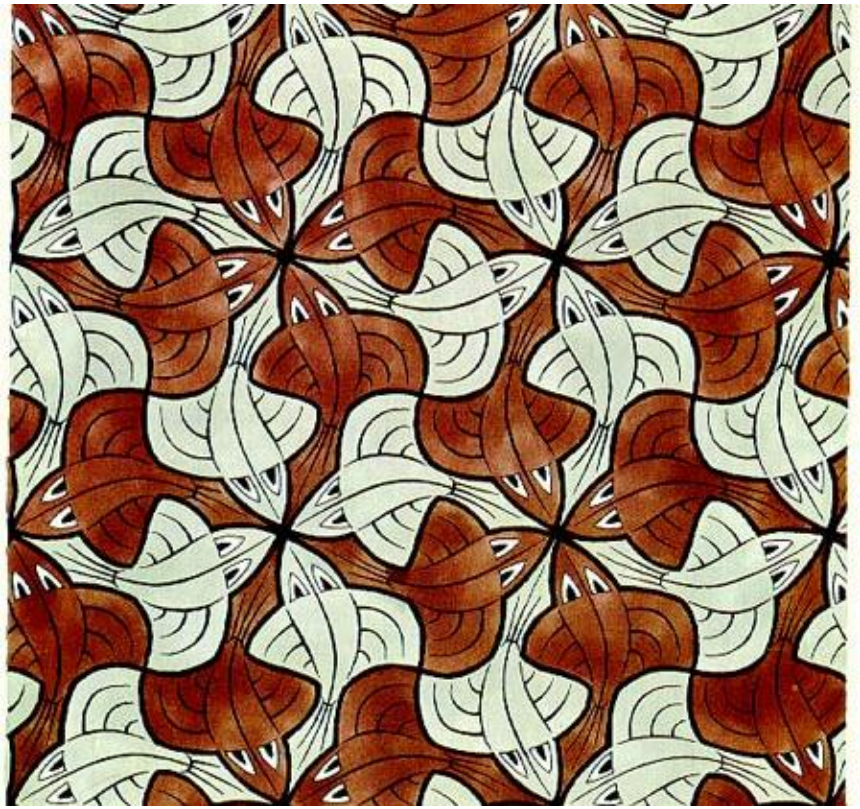
all crystals have **TRANSLATIONAL SYMMETRY**….





…and most also have **ROTATIONAL SYMMETRY.**

Images: M.C. Escher

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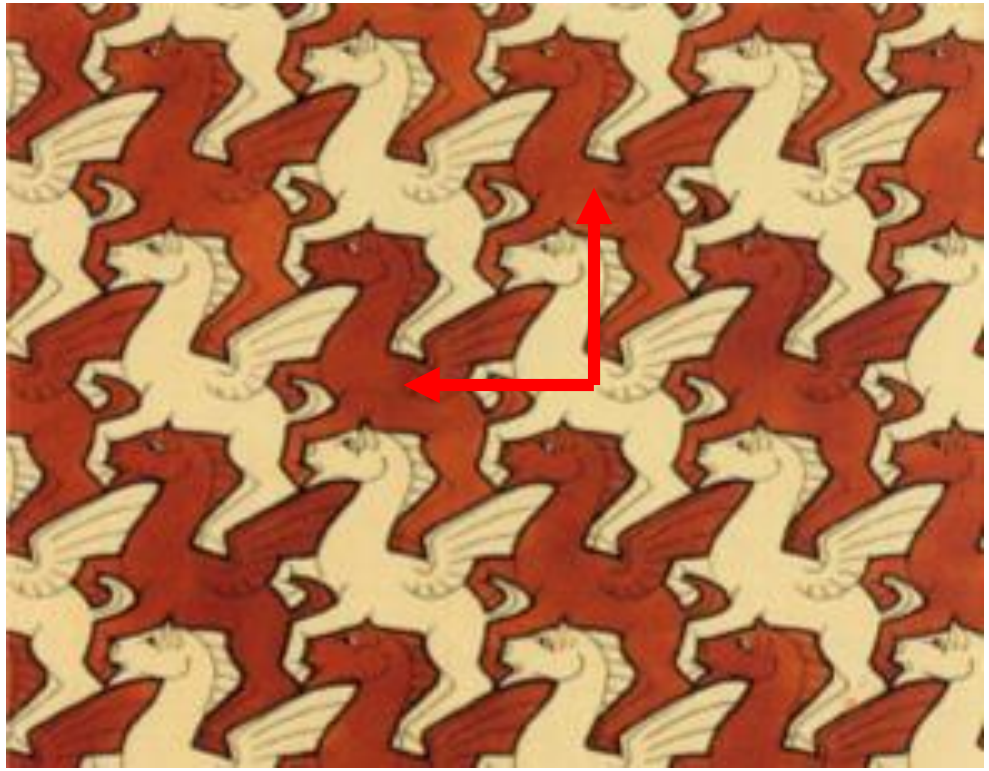
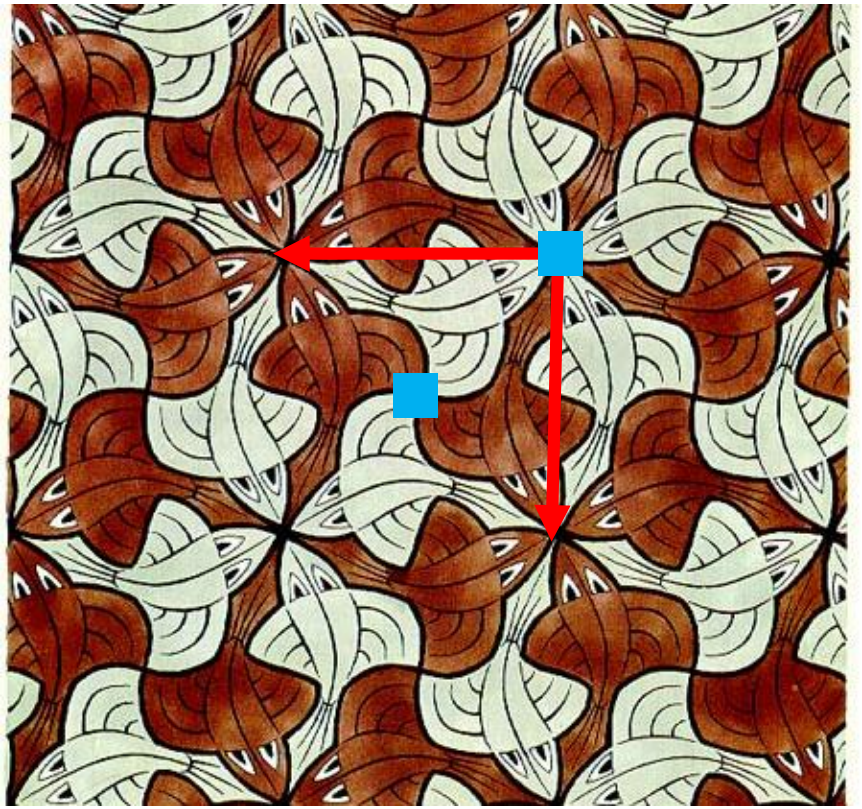




…and most also have **ROTATIONAL SYMMETRY.**

***2-, 3-, 4-, or 6-fold rotational symmetry (only!)***

Images: M.C. Escher

# Some Definitions

- **Unit Cell (cell)**
  - The unit cell completely defines the symmetry and structure of the entire crystal lattice, which is built up by repetitive translation of the unit cell along its principal axes.

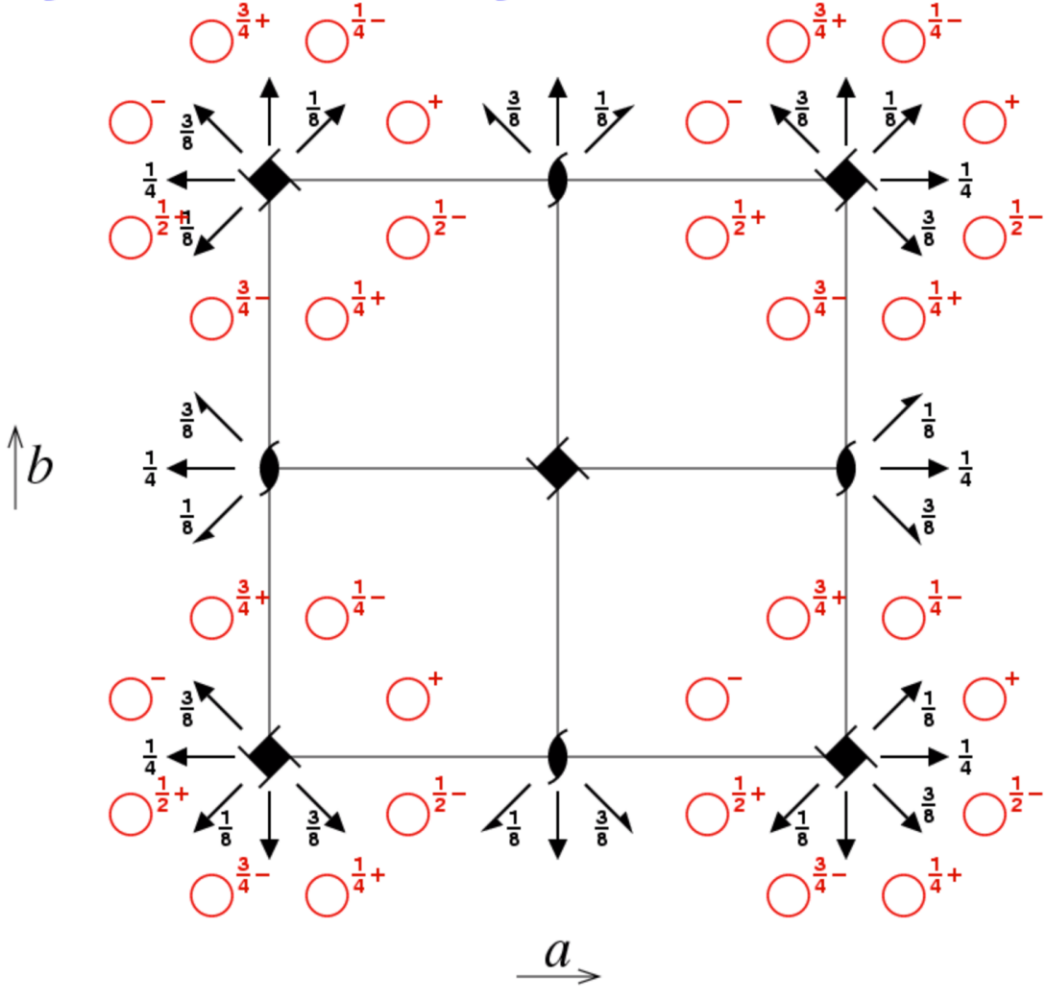
- **Space Group (SG)**
  - Mathematical group of symmetry operations that gives rise to one of the general arrangements of motifs in a 3-dimensional periodic crystal structure. (i.e. A specific set of rotational symmetry operations that preserves the translational symmetry of the crystal.)
  - There are a finite number of ways to arrange motifs in a crystal:
    - 230 possible space groups, but only 65 apply to chiral molecules (biomolecules).
    - The 65 SGs we care about contain rotation and “screw” operations. No mirror, “glide,” or inversion operations.

- **Asymmetric Unit (ASU)**
  - Smallest part of a crystal structure, containing the motif. Application of space group symmetry operations to the ASU generates a periodic crystal structure.
  - One Hsp90 molecule (+/- ADP, or fragment, etc.) for *most* of our crystals

# Space Group for our Hsp90 Crystals:

img.chem.ucl.ac.uk/sgp/large/095az1.htm

$P4_322$ $P\,4_3\,2\,2$ 422 No. 95




1 $x, y, z$

2 $\bar{x}, \bar{y}, \frac{1}{2} + z$

3 $\bar{y}, x, \frac{3}{4} + z$

4 $y, \bar{x}, \frac{1}{4} + z$

5 $x, \bar{y}, \frac{1}{2} - z$

6 $\bar{x}, y, \bar{z}$

7 $\bar{y}, \bar{x}, \frac{3}{4} - z$

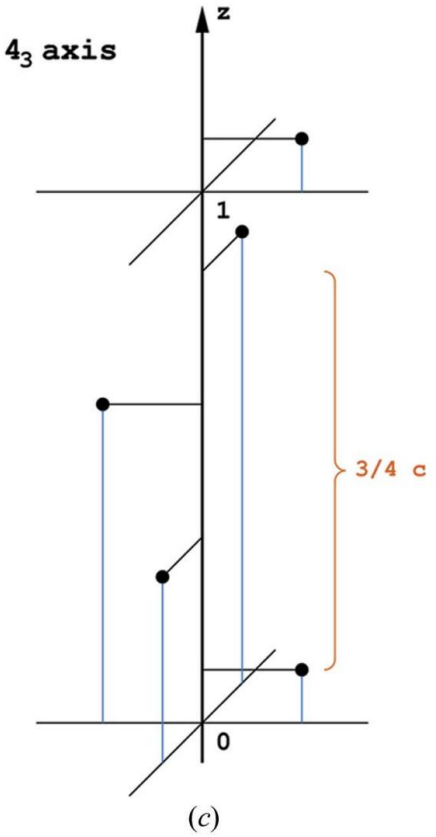
8 $y, x, \frac{1}{4} - z$

# Let's Break Down $P4_322$

- Symmetry Operations:
  - Three mutually perpendicular symmetry "generators":
    - $4_3$ screw axis
    - Two 2-fold rotation axes

What's a $4_3$ screw axis?

- Rotate 90° CCW and translate along rotation axis by ¾ of unit cell length.

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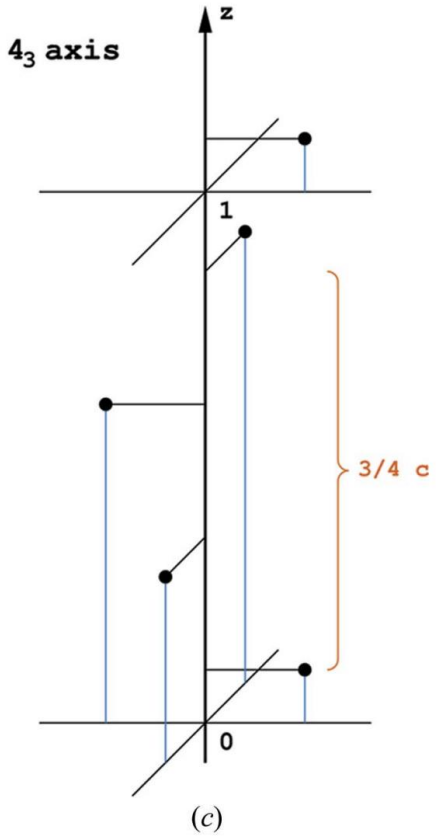


First copy at x

90° -> x +¾

180° -> x +1½ = x +½

270° -> x +2¼ = x +¼

360° = back to x

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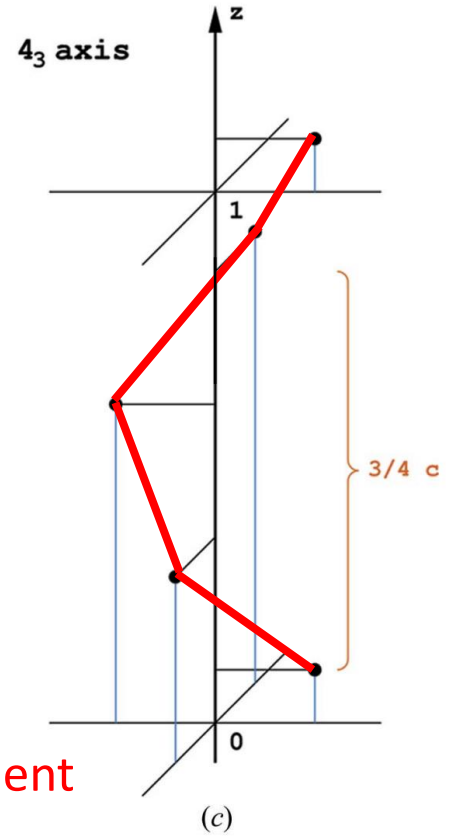


First copy at **x**

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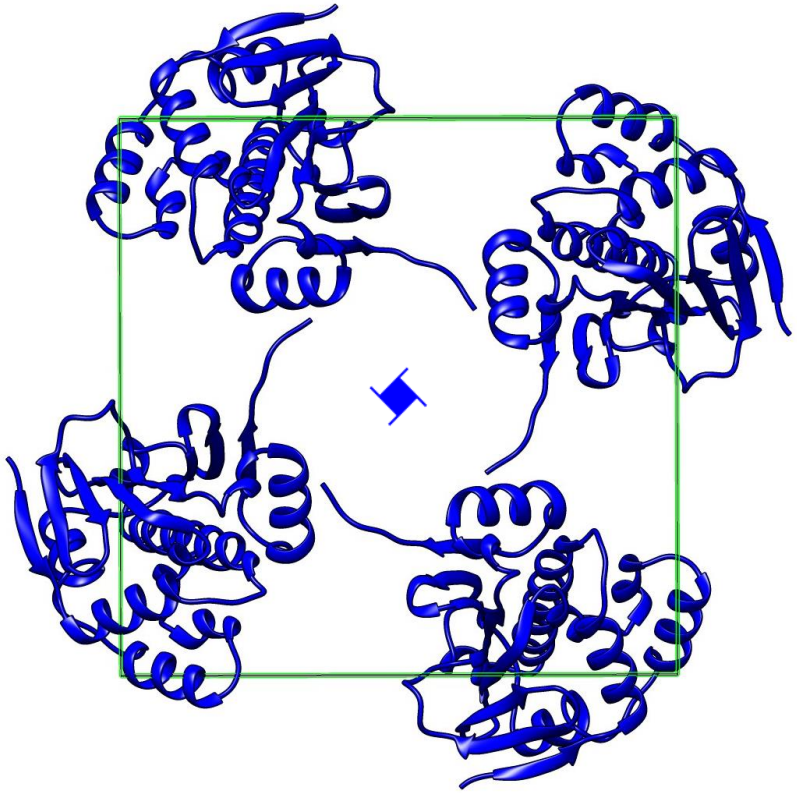
360 = back to x

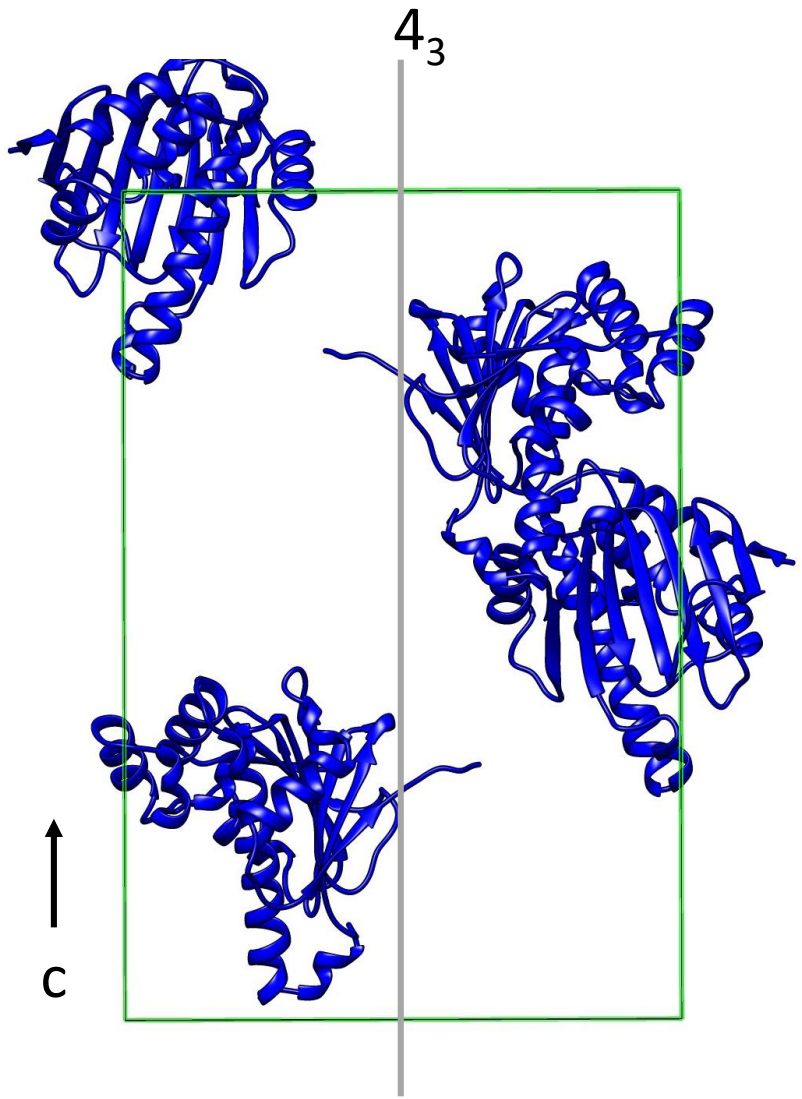
A left handed helical arrangement

Dauter and Jaskolski (2010) J. Appl. Cryst.

# A $4_3$ Screw Axis in the Unit Cell



a = b



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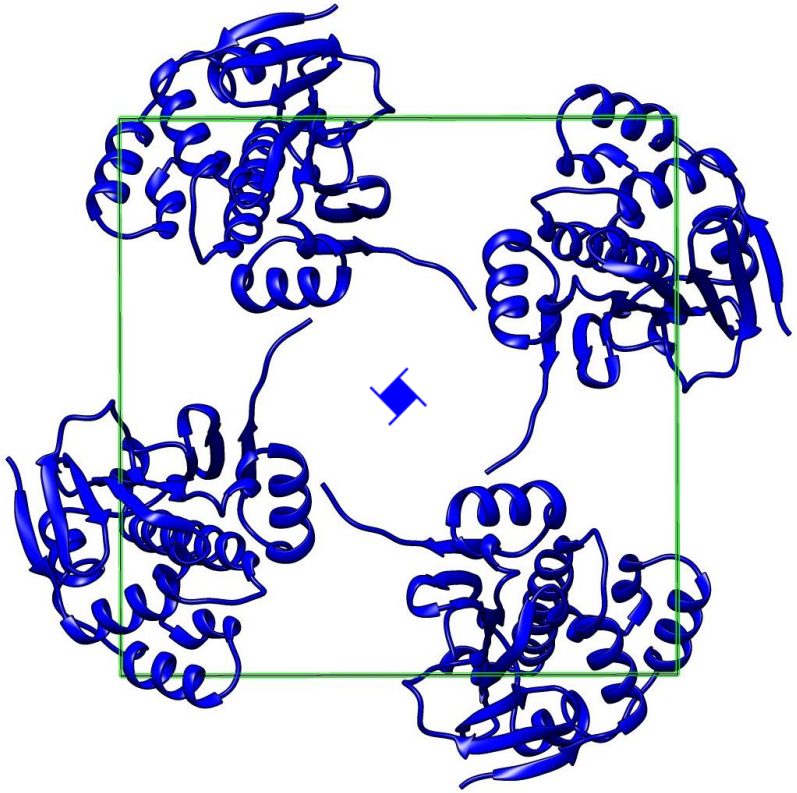
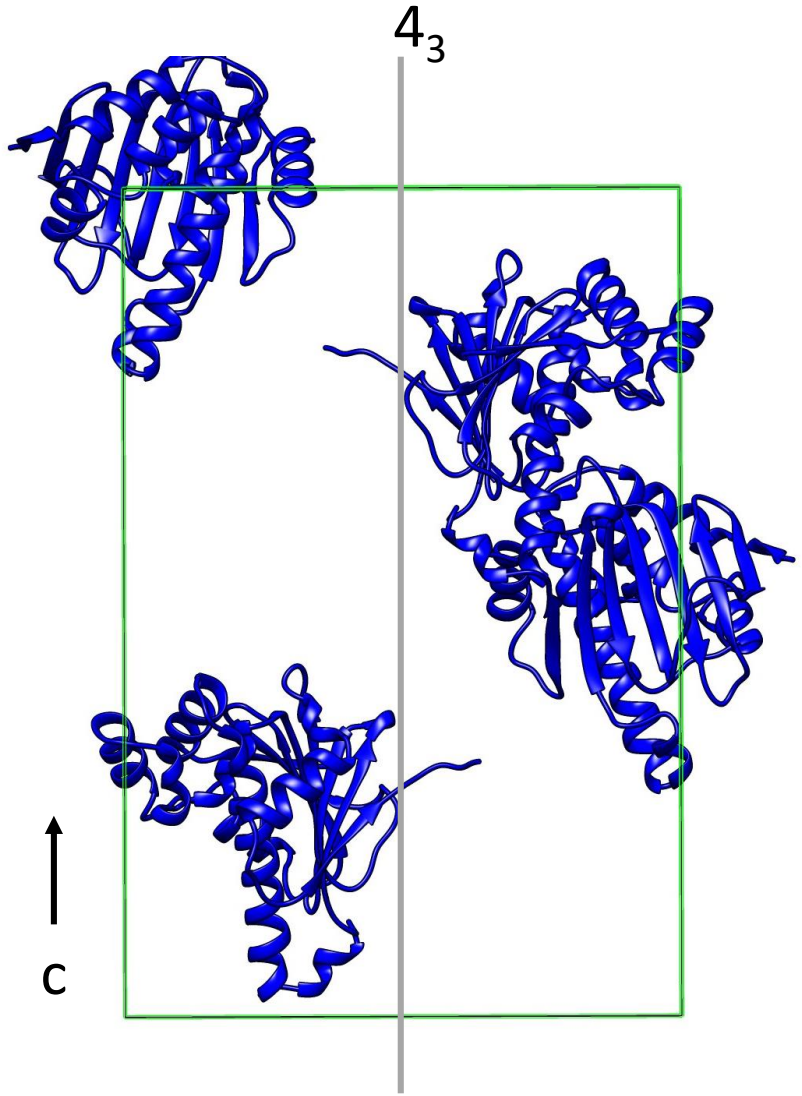
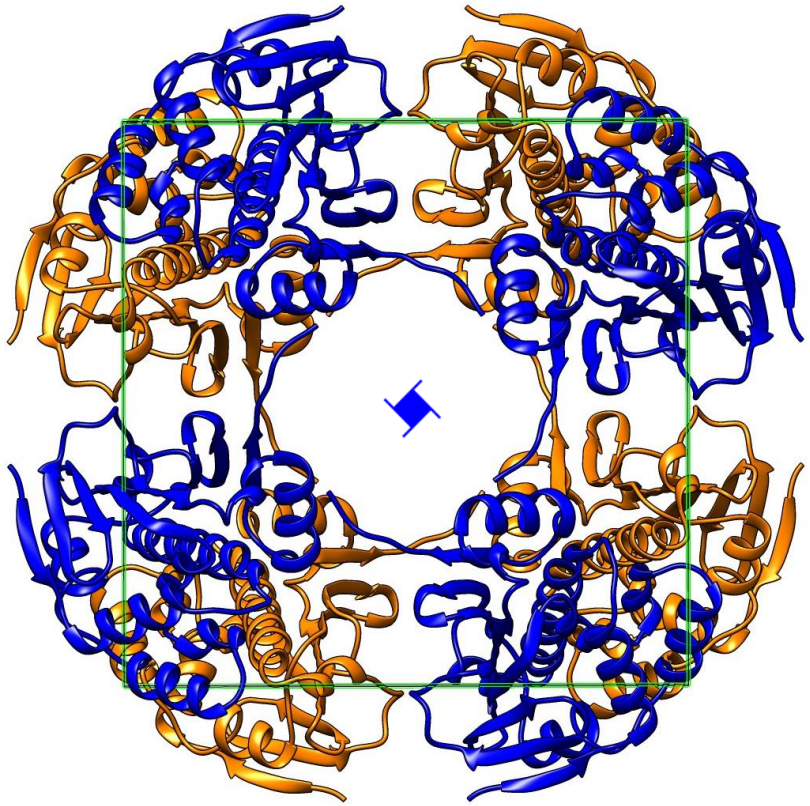


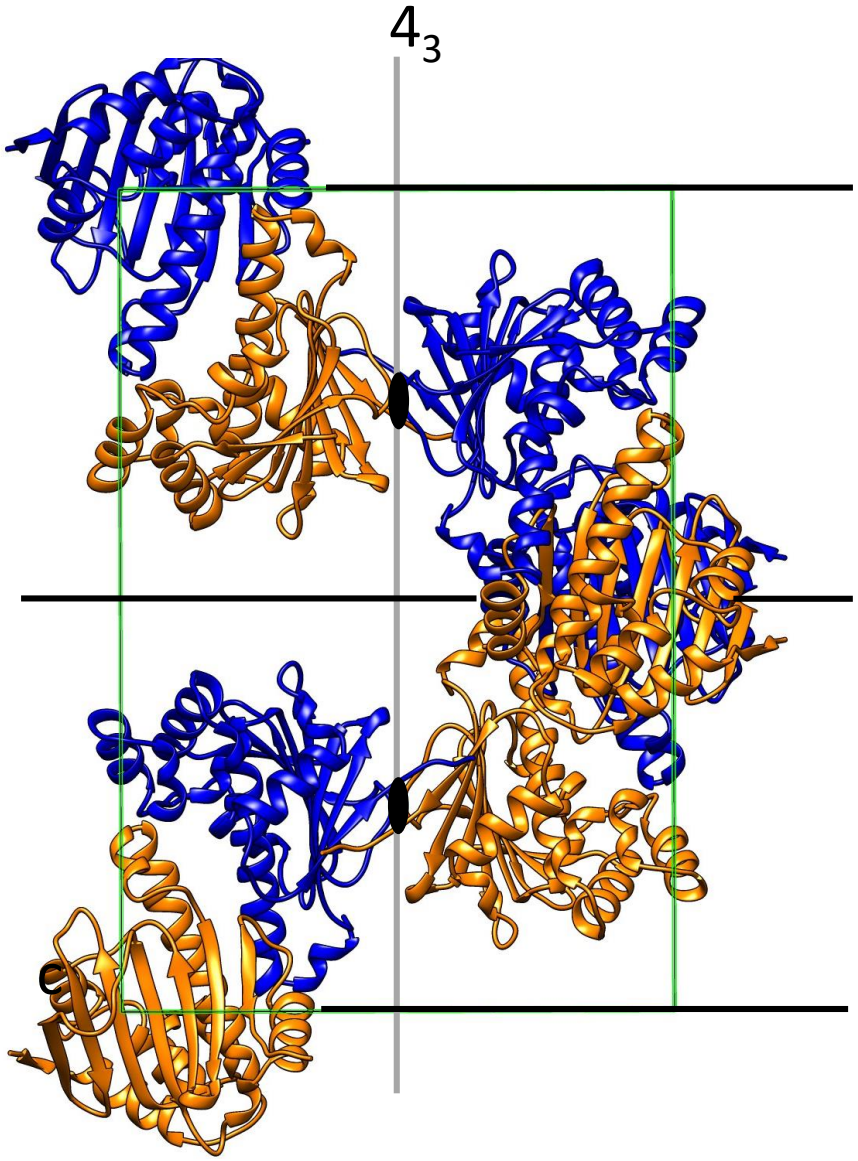
a = b




But this crystal is not packed completely. There are gaps between molecules.

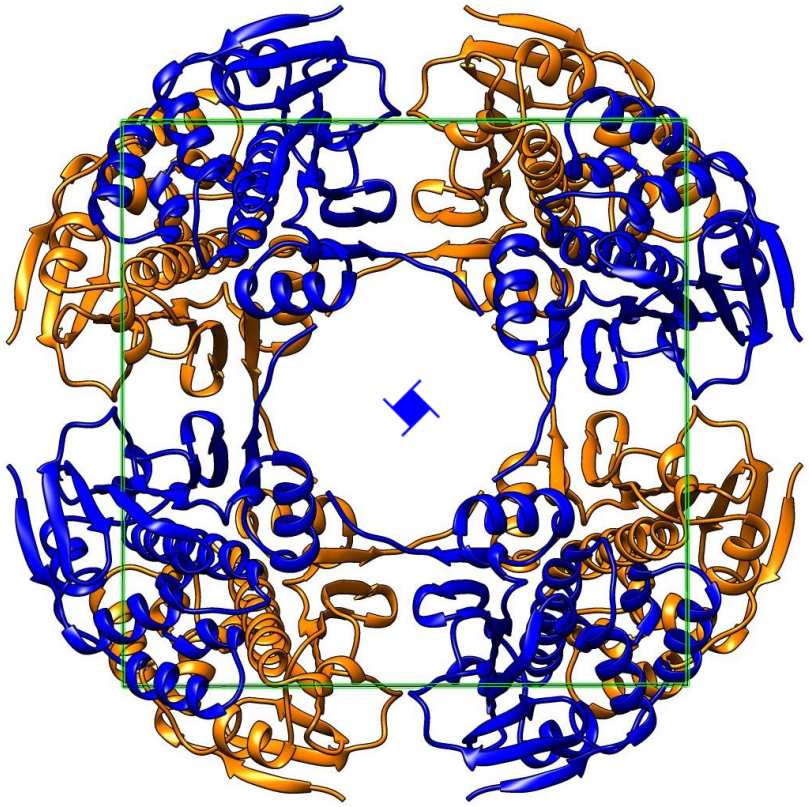
# Introducing 2-fold Symmetry Completes Unit Cell Packing

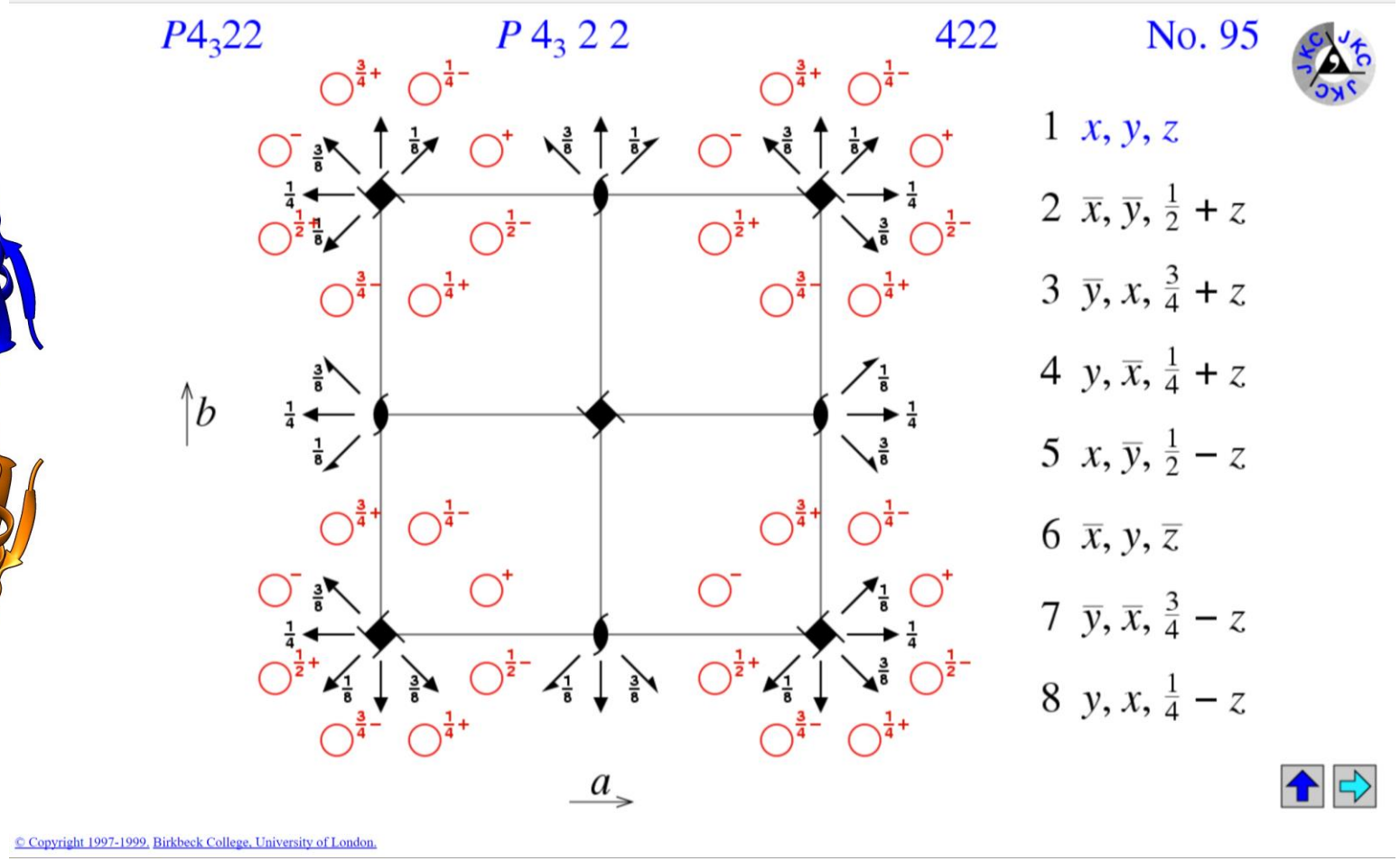





Additional 2-fold symmetry operations – four of them, related by the $4_3$ screw – fill out the unit cell.
There are eight molecules (ASUs) in the unit cell.

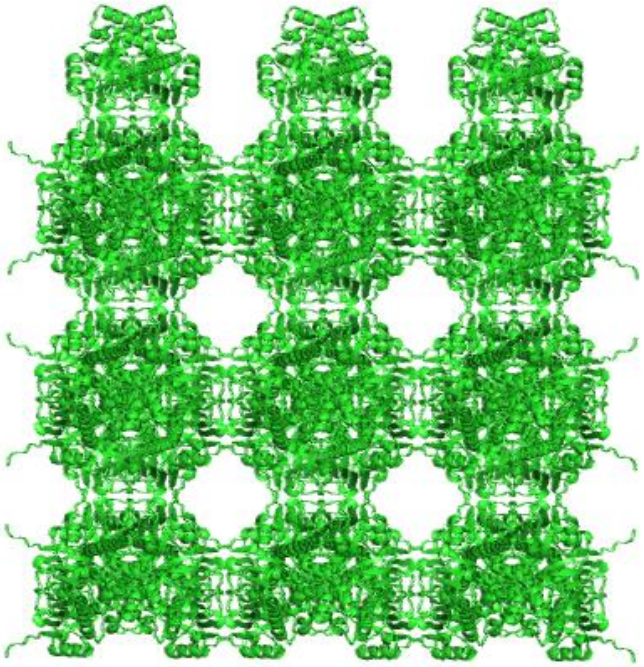
# Makes a Little More Sense Now?

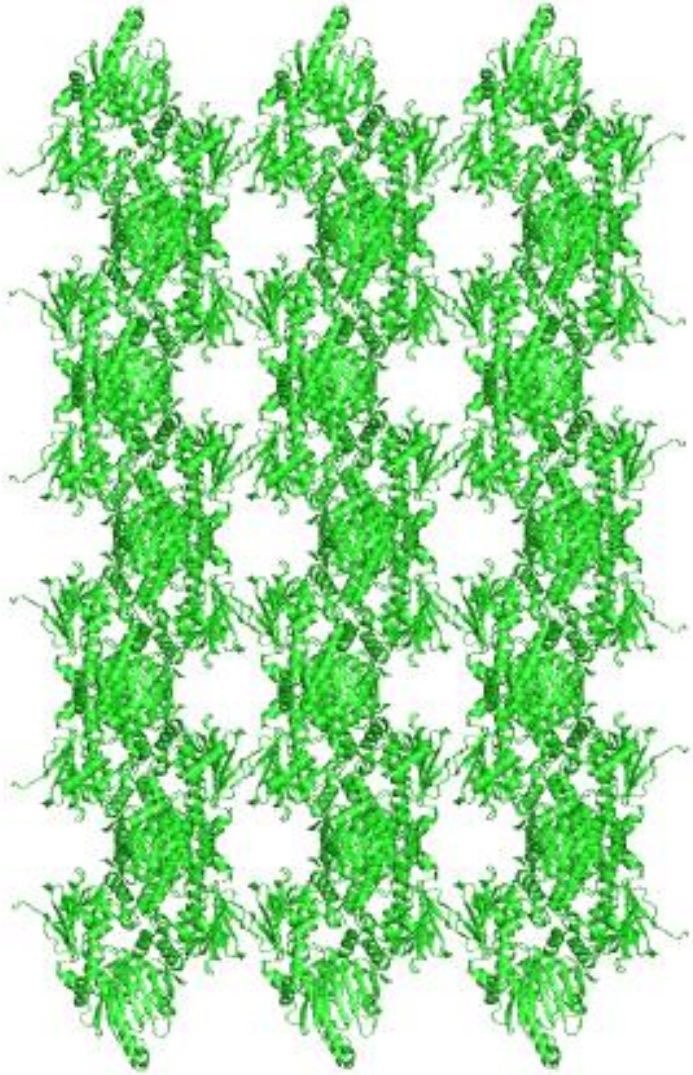





To learn more about space group symmetry and diagrams, check out: Dauter and Jaskolski (2010) J. Appl. Cryst.

# Rotational and Translational Symmetry Build A Crystal from a Unit Cell





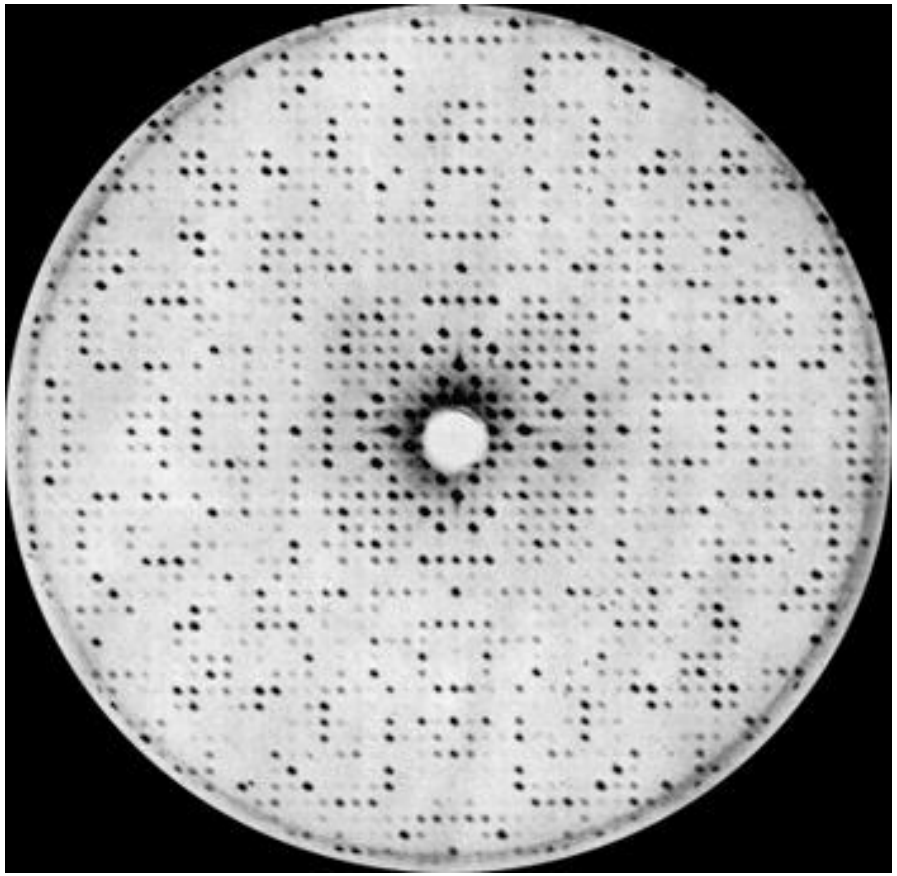
A typical crystal contains $10^9$-$10^{12}$ molecules. Also note the large solvent channels, which facilitate ligand soaking.

**But We Just Cheated!!!**

**I showed you the packing for a crystal structure we haven't determined yet.**

**In practice, we need to figure out the space group before we determine the structure.**

# Space Group Symmetry Results in Symmetric Diffraction Patterns



A “precession photograph” taken from a lysozyme crystal shows a slice (h,k,0) of reciprocal space.

The pattern of reflection intensities in reciprocal space has symmetry related to the space group symmetry.

- Symmetry of molecular packing plus an inversion (-x,-y,-z) operation.
- Laue Symmetry

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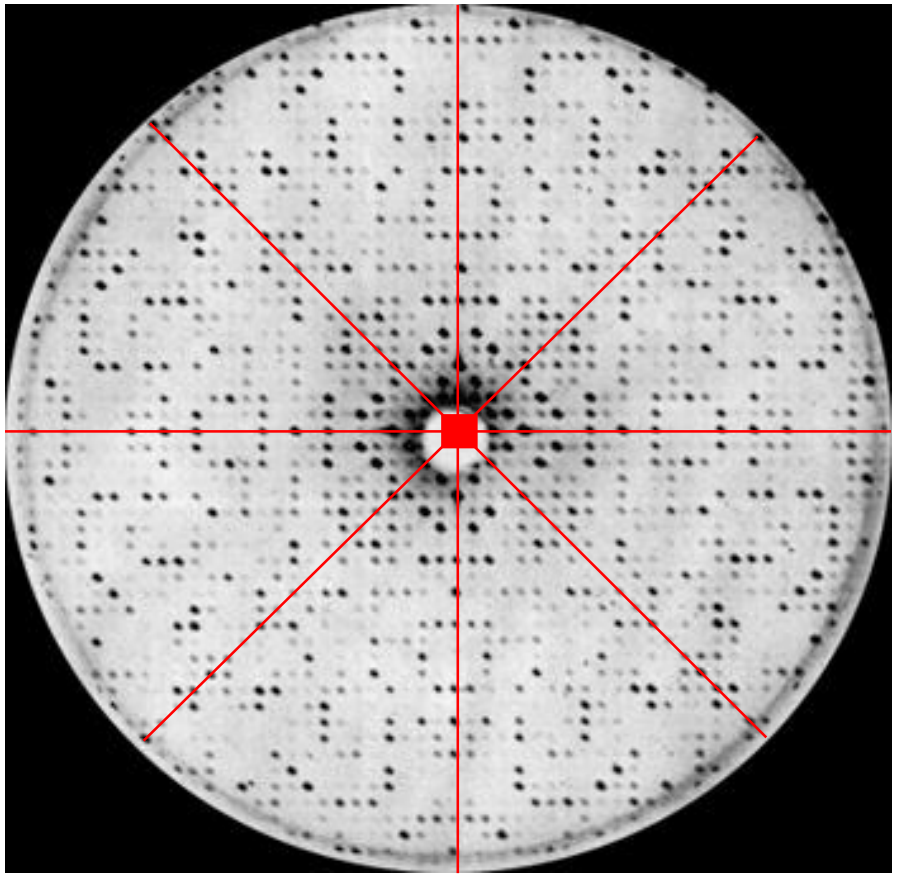

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- Symmetry of molecular packing plus an inversion (-x,-y,-z) operation.
- Laue Symmetry

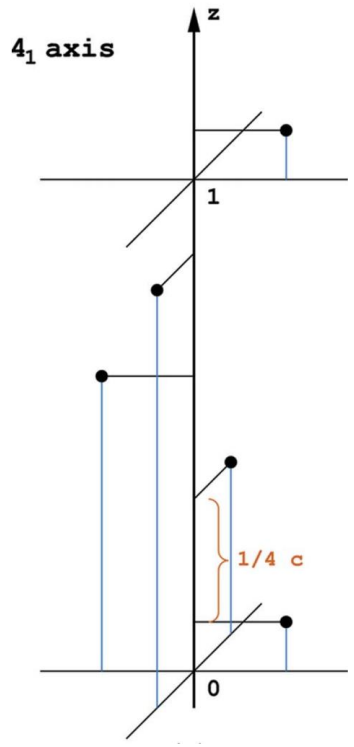
- For $P4_322$, Laue symm is 4/mmm
  - Hsp90 and Lysozyme have the same symmetry

- If the crystal is perfectly oriented, we only need to rotate it 22.5° to measure all unique reflections once.

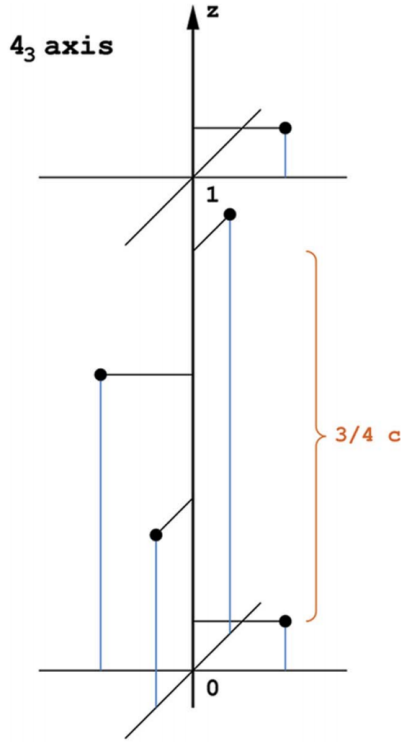
# Ambiguity in Space Group Assignment – $P4_322$ vs. $P4_122$

- The symmetry of the diffraction pattern tells us about rotational symmetry in the crystal, but some ambiguities about symmetry elements remain.

- The diffraction alone cannot differentiate between $4_3$ and $4_1$ screw axes.
  - Enantiomorphs or “handedness.”




90° rotation and
+¼ translation

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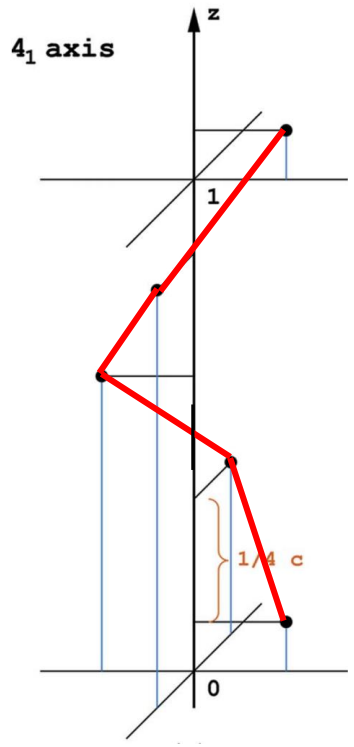
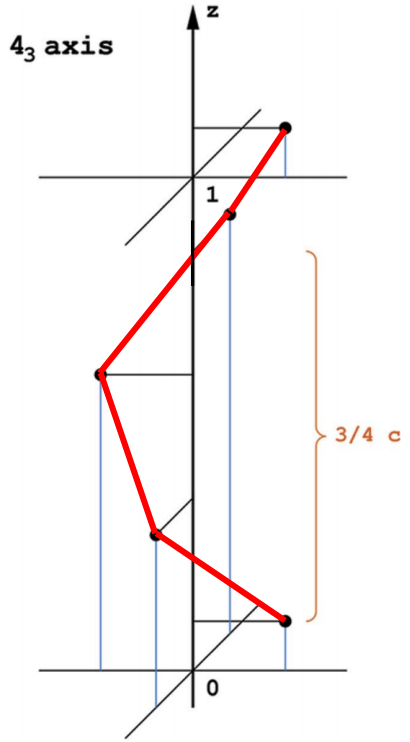



90° rotation and
+¼ translation

Right handed helical arrangement

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Left handed helical arrangement

Dauter and Jaskolski (2010) J. Appl. Cryst.

# Ambiguity in Space Group Assignment – $P4_322$ vs. $P4_122$

- The symmetry of the diffraction pattern tells us about rotational symmetry in the crystal, but some ambiguities about symmetry elements remain.

- The diffraction alone cannot differentiate between 43 and 41 screw axes.
  - Enantiomorphs or “handedness.”

- **So when you process your data, you might get either result. For our purposes, the ambiguity is resolved by trying both during molecular replacement phasing.**

# Sometimes Things Can Get Complicated…

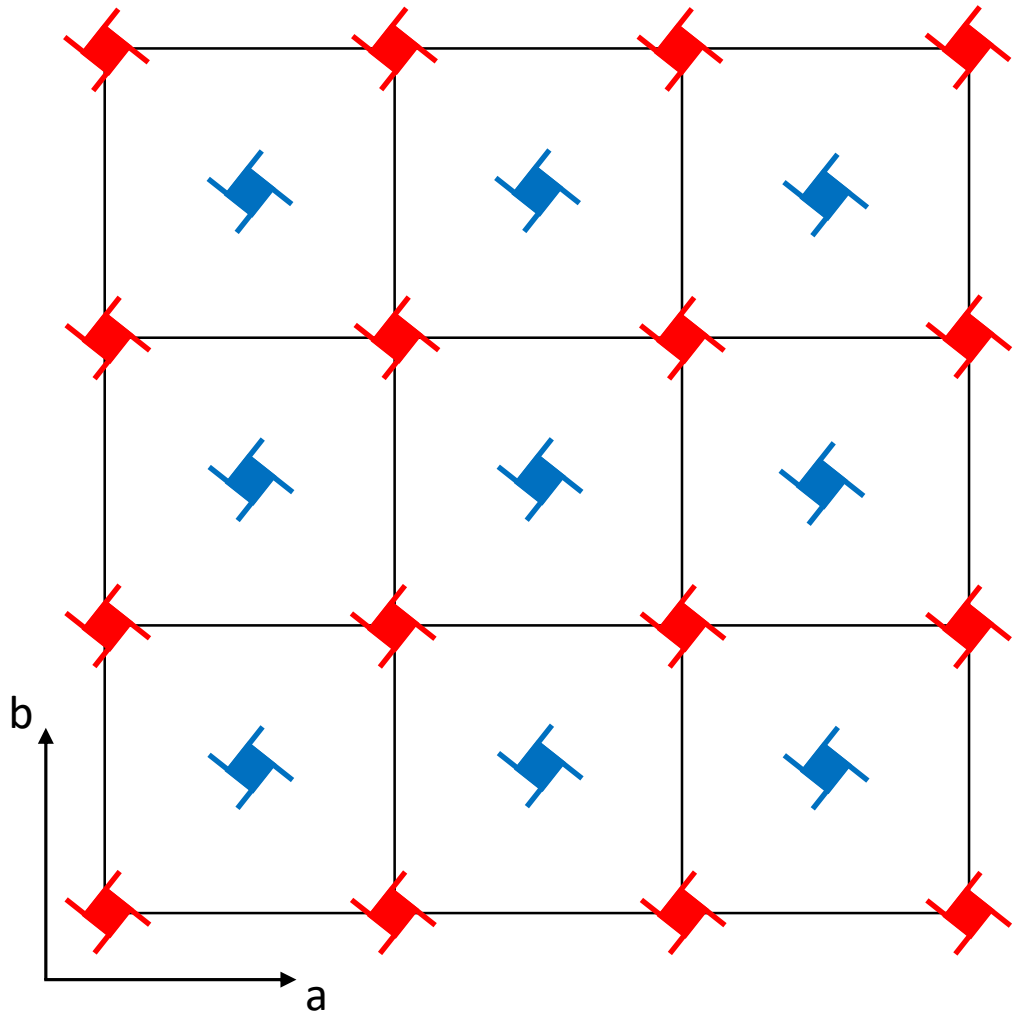
- You may find some datasets with a larger unit cell (2x volume).
  - How?
  - Why?

*Small (normal) unit cell:*

a=b=75Å, c=109Å, α=β=γ=90°

*Large unit cell:*

a=b=104Å, c=109Å, α=β=γ=90°



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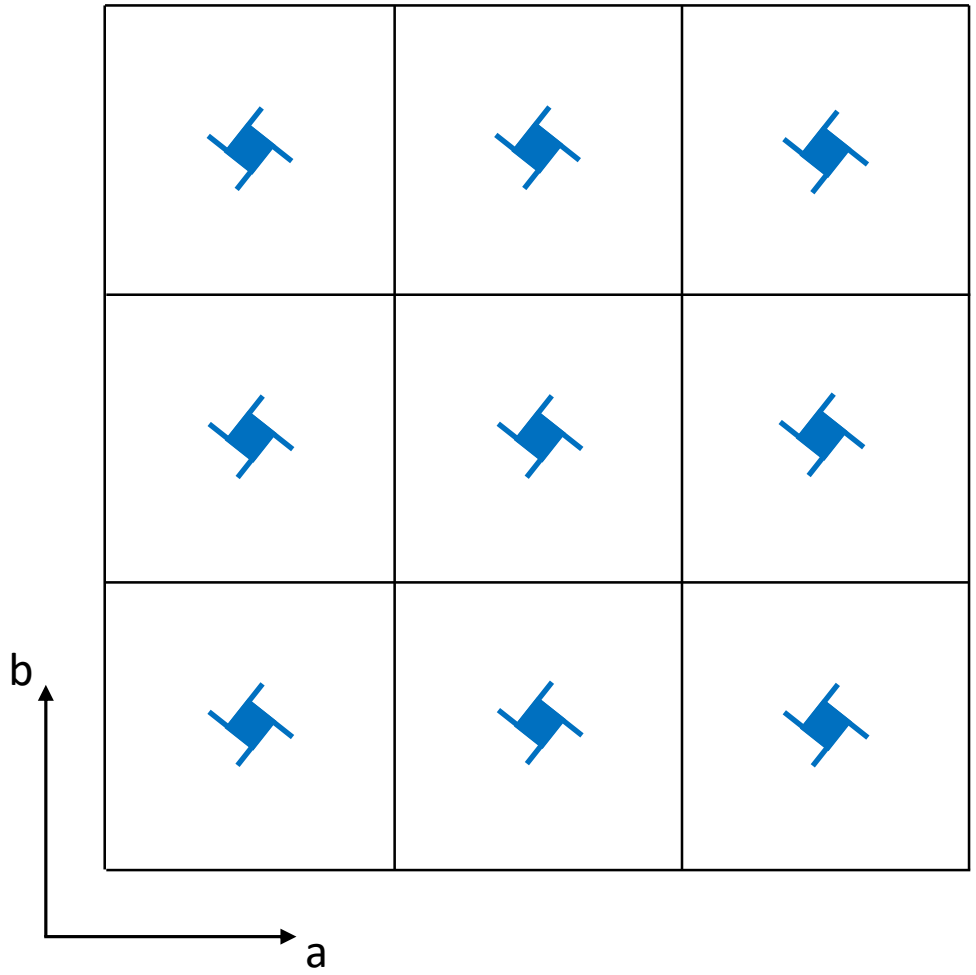

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- You may find some datasets with a larger unit cell (2x volume).
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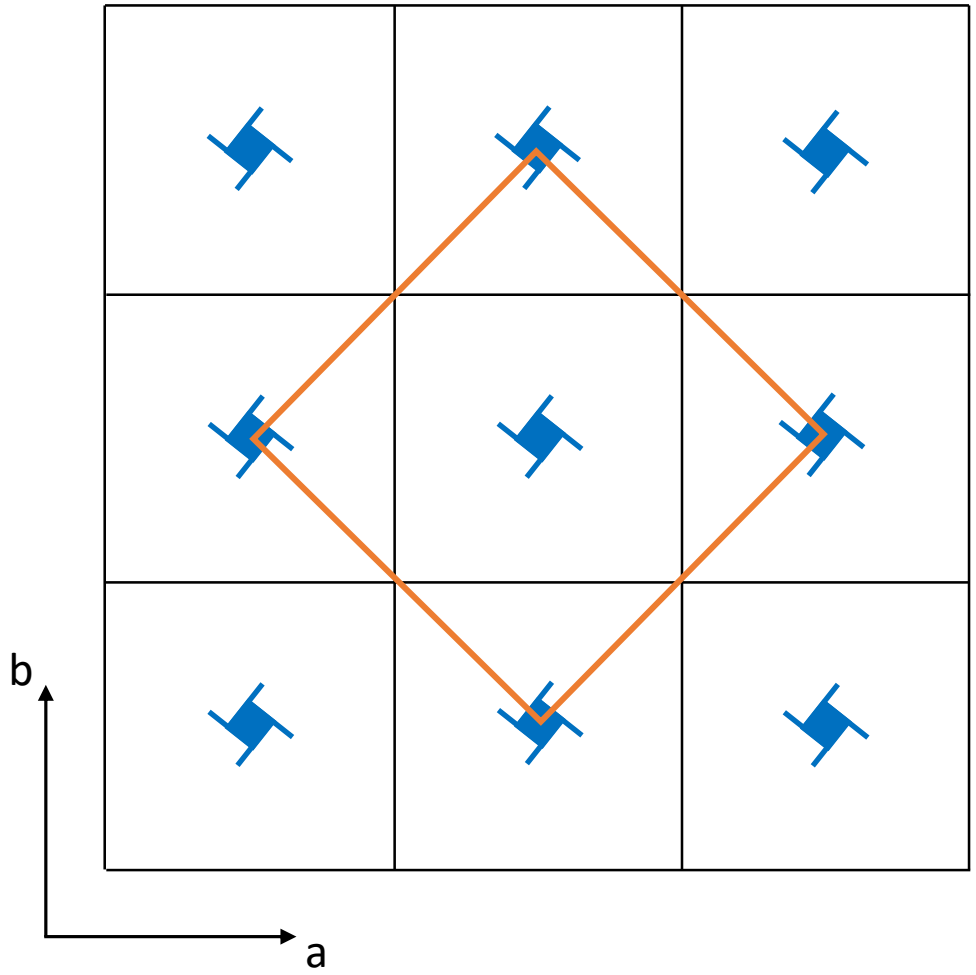

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**75Å * $\sqrt{2}$ = 104Å**

**When processing X-ray data, be mindful of geometric relationships and symmetry groups.**