# Symmetries

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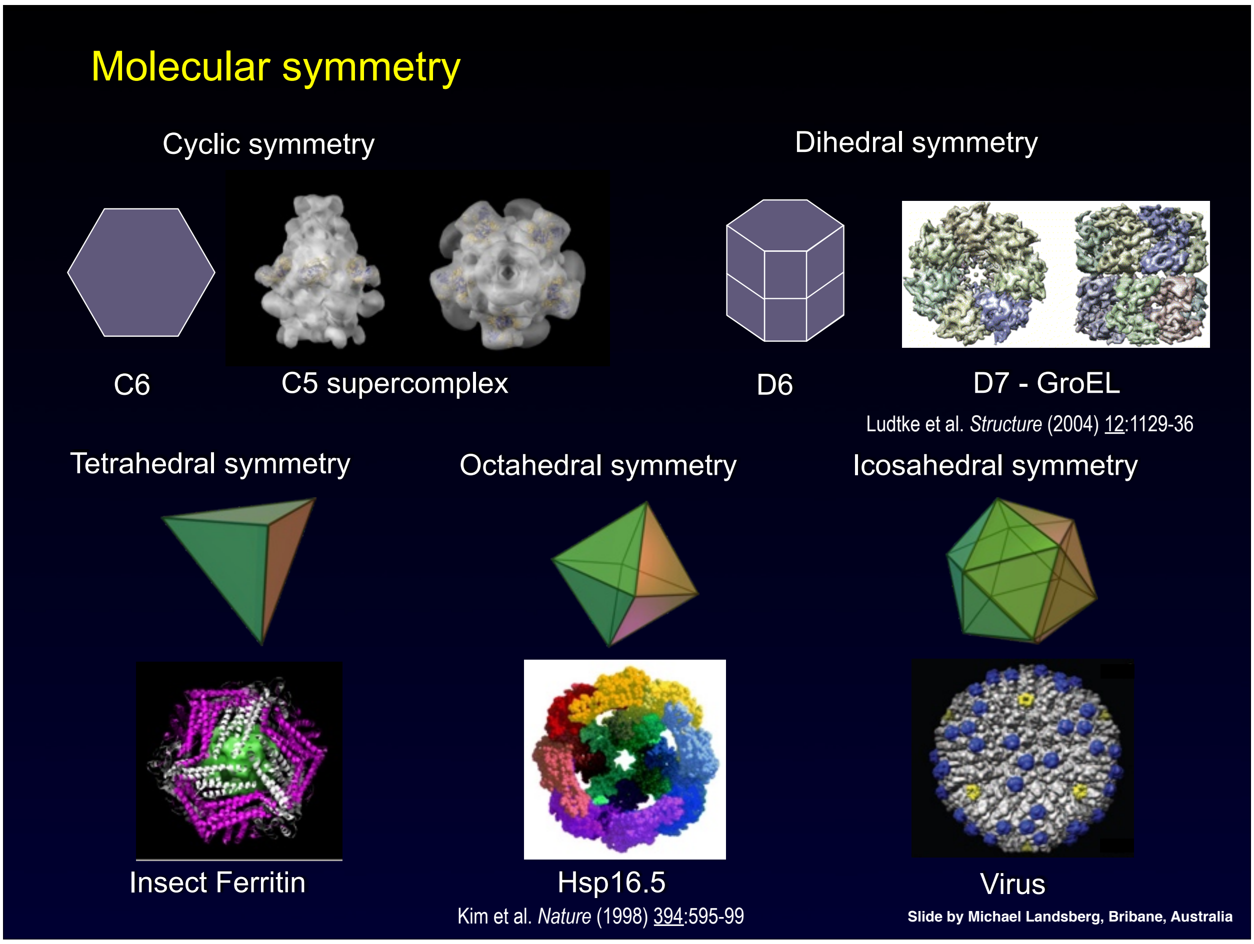


# Plane group notation

## Hermann-Mauguin style

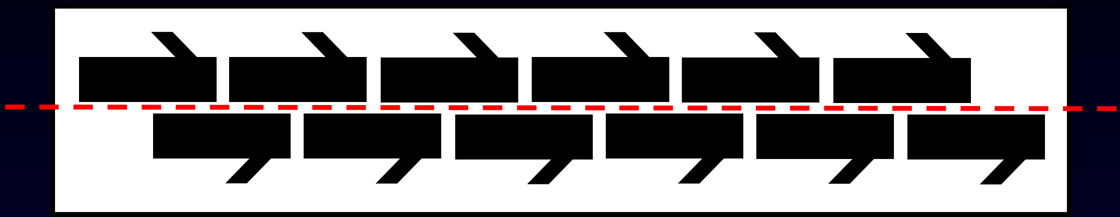
- Begins with either *p* or *c*, for a primitive cell or a face-centered cell
- This is followed by a digit, *n*, indicating the highest order of rotational symmetry: 1-fold (none), 2-fold, 3-fold, 4-fold, or 6-fold
- The next two symbols indicate symmetries relative to the "main" translation axis of the pattern; if there is a mirror perpendicular to a translation axis this is the main one (or if there are two, one of them).
  - The symbols are either *m*, *g*, or *1*, for mirror, glide reflection, or none.
  - The axis of the mirror or glide reflection is perpendicular to the main axis for the first letter…
  - …and either parallel or tilted 180°/*n* (when *n* > 2) for the second letter.

***p2mg***



# Translation + Reflection = Glide Reflection

**Translation by ½ unit cell combined with a reflection about a line parallel to the direction of translation**



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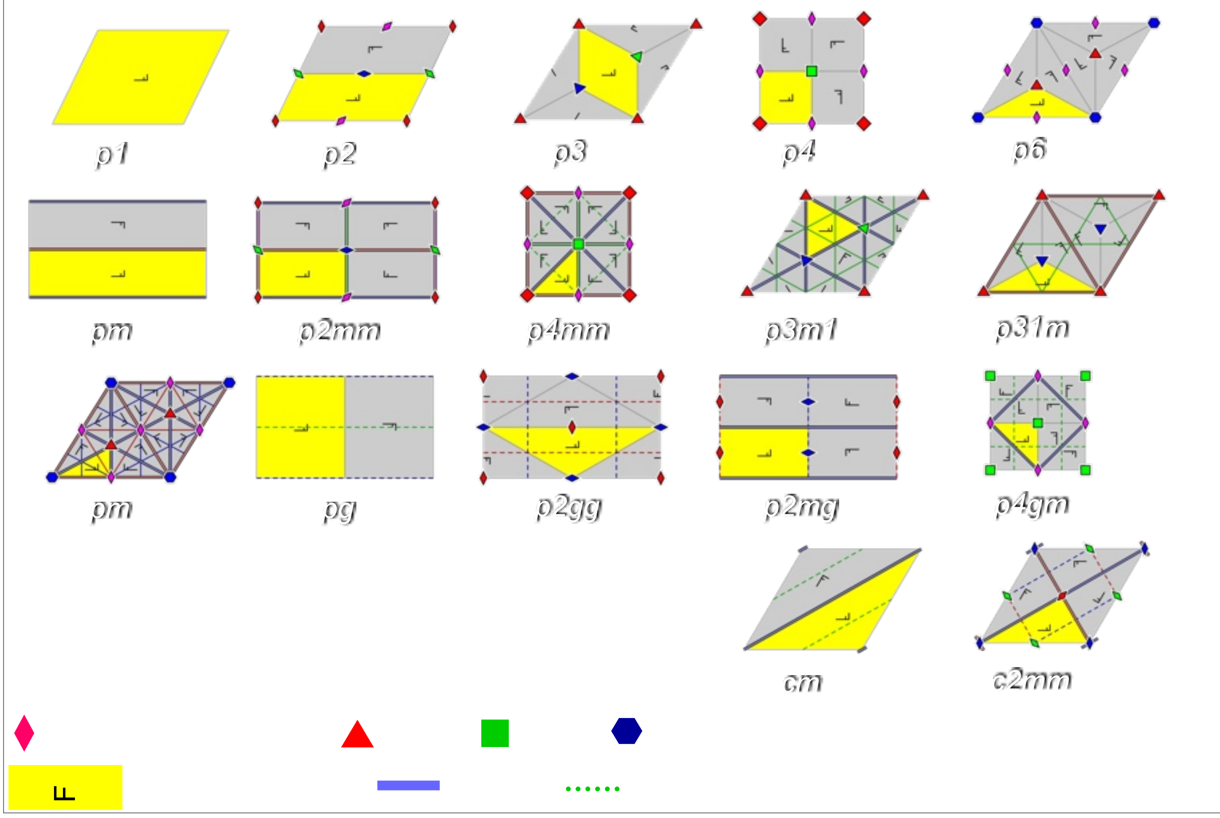
## Plane group definitions






## Group theory

- A crystallographic *space group* is the mathematical group of symmetry operations which apply to both the given unit cell and the crystal array
- There are 230 possible crystallographic space groups in 3D
  - 65 for proteins and chiral molecules
- *17 plane groups* describe all the possible symmetry arrangements in projection images of 2D crystals
- These plane groups are different (but correlate somewhat trivially) to the 17 2D *space groups* which describe all possible 2D crystal arrangements

# Symmetry of 2D crystals

| Two-sided Plane Group* | Corresponding 3-dimensional space group | Projection Symmetry |
|---|---|---|
| p1 | P1 | p1 |
| p21 | P2(c-axis unique) | p2 |
| p12 | P2(b-axis unique) | pm |
| $p12_1$ | $P2_1$ | pg |
| c12 | C2 | cm |
| p222 | P222 | pmm |
| $p222_1$ | $P222_1$ | pmg |
| $p22_12_1$ | $P22_12_1$ | pgg |
| c222 | C222 | cmm |
| p4 | P4 | p4 |
| p422 | P422 | p4m |
| $p42_12$ | $P42_12$ | p4g |
| p3 | P3 | p3 |
| p312 | P312 | p3m1 |
| p321 | P321 | p31m |
| p6 | P6 | p6 |
| p622 | P622 | p6m |

* We use here the nomenclature for the two-sided plane groups proposed by Holser (1958). This nomenclature has the following main rules.

(a) Cell type is indicated first by a small letter, p or c.

(b) The axis perpendicular to the plane is always chosen as the z-axis.

(c) The symmetry along this axis is always described by the first symbol following the cell type.

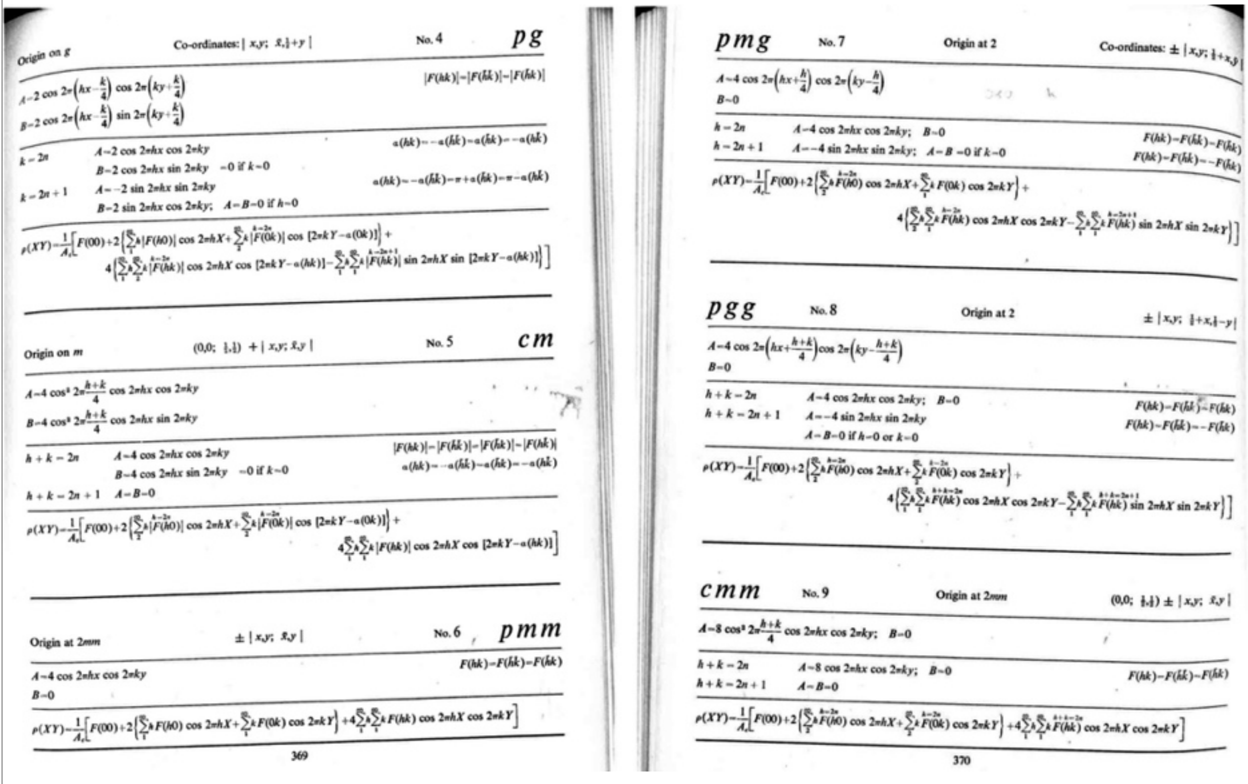
† There are 80 two-sided plane groups in total, of which the 17 given here are the only ones not containing inversion centres or mirror or glide planes.



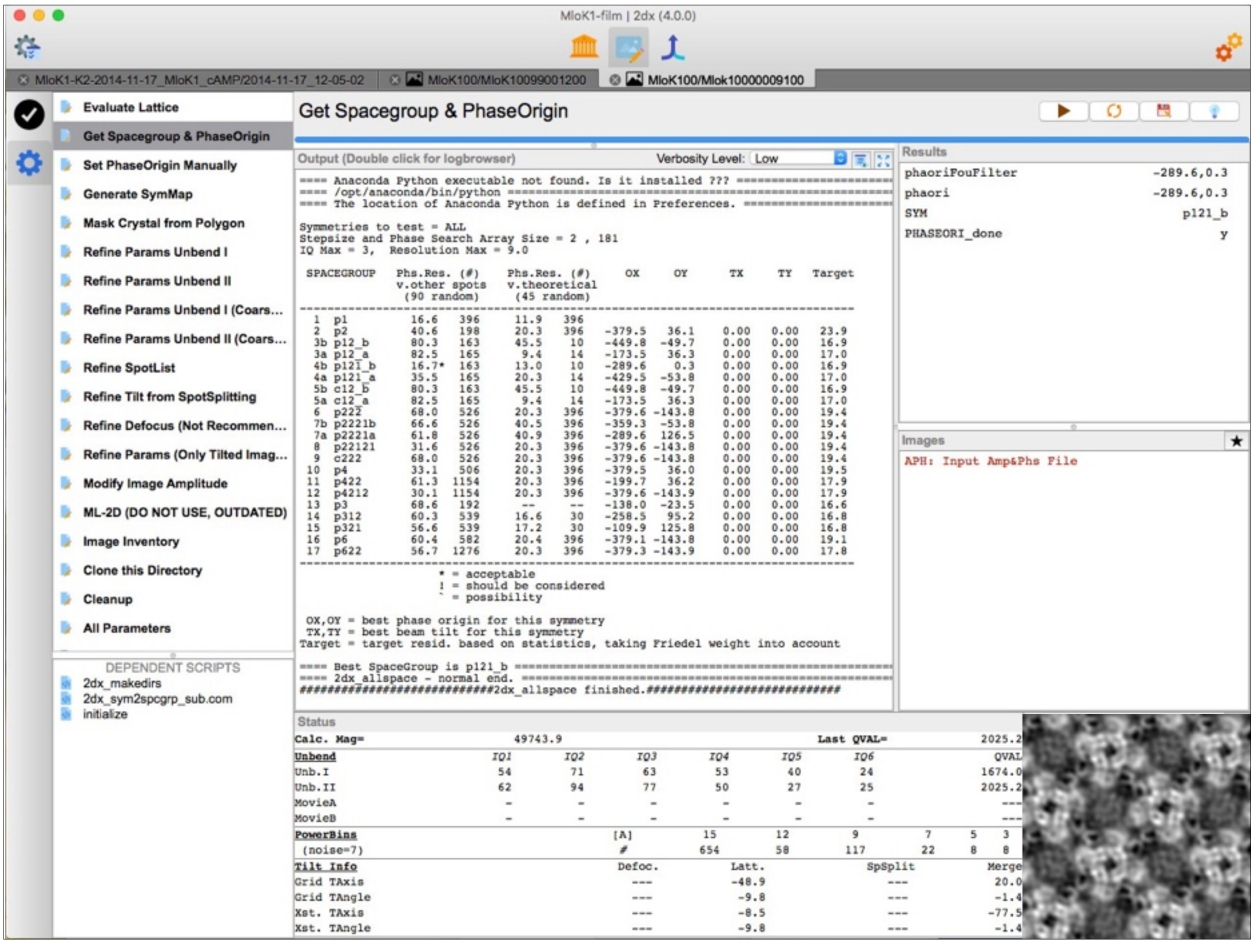
# Symmetry of 2D crystals

1. An electron micrograph is a projection of the object along the direction of the electron beam.
2. Two-dimensional plane groups describe the projection symmetry, 17 possibilities. Listed in the Int Tab for X-ray Crystallography.
3. The specimen has an extension in the third dimension ("top and bottom").
4. Two-sided plane groups describe the symmetry of 2D crystals, 17 possibilities for biological molecules.
5. The smallest repeating unit, the unit cell is described by the lattice vectors a and b and the angle gamma between them.
6. Depending on the symmetry, the unit cell may contain multiple copies of the molecule.
7. In addition, non-crystallographic symmetry may add even more molecules to the unit cell.
8. The packing arrangement in a 2D crystal can give information about oligomeric arrangement of the protein.

# Symmetry of 2D crystals





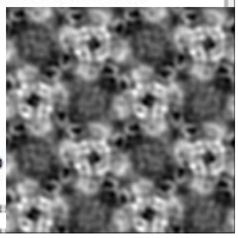



```
Symmetries to test = ALL
Stepsize and Phase Search Array Size = 2 , 181
IQ Max = 3,  Resolution Max = 9.0

 SPACEGROUP   Phs.Res. (#)     Phs.Res. (#)     OX        OY       TX       TY      Target
              v.other spots    v.theoretical
               (90 random)      (45 random)
-------------------------------------------------------------------------------------------
   1  p1        16.6    396      11.9    396
   2  p2        40.6    198      20.3    396    -379.5    36.1    0.00     0.00     23.9
   3b p12_b     80.3    163      45.5     10    -449.8   -49.7    0.00     0.00     16.9
   3a p12_a     82.5    165       9.4     14    -173.5    36.3    0.00     0.00     17.0
   4b p121_b    16.7*   163      13.0     10    -289.6     0.3    0.00     0.00     16.9
   4a p121_a    35.5    165      20.3     14    -429.5   -53.8    0.00     0.00     17.0
   5b c12_b     80.3    163      45.5     10    -449.8   -49.7    0.00     0.00     16.9
   5a c12_a     82.5    165       9.4     14    -173.5    36.3    0.00     0.00     17.0
   6  p222      68.0    526      20.3    396    -379.6  -143.8    0.00     0.00     19.4
   7b p2221b    66.6    526      40.5    396    -359.3   -53.8    0.00     0.00     19.4
   7a p2221a    61.8    526      40.9    396    -289.6   126.5    0.00     0.00     19.4
   8  p22121    31.6    526      20.3    396    -379.6  -143.8    0.00     0.00     19.4
   9  c222      68.0    526      20.3    396    -379.6  -143.8    0.00     0.00     19.4
  10  p4        33.1    506      20.3    396    -379.5    36.0    0.00     0.00     19.5
  11  p422      61.3   1154      20.3    396    -199.7    36.2    0.00     0.00     17.9
  12  p4212     30.1   1154      20.3    396    -379.6  -143.9    0.00     0.00     17.9
  13  p3        68.6    192       --      --    -138.0   -23.5    0.00     0.00     16.6
  14  p312      60.3    539      16.6     30    -258.5    95.2    0.00     0.00     16.8
  15  p321      56.6    539      17.2     30    -109.9   125.8    0.00     0.00     16.8
  16  p6        60.4    582      20.4    396    -379.1  -143.8    0.00     0.00     19.1
  17  p622      56.7   1276      20.3    396    -379.3  -143.9    0.00     0.00     17.8
-------------------------------------------------------------------------------------------
                          * = acceptable
                          ! = should be considered
                          ` = possibility

 OX,OY = best phase origin for this symmetry
 TX,TY = best beam tilt for this symmetry
Target = target resid. based on statistics, taking Friedel weight into

==== Best SpaceGroup is p121_b ==========================================
==== 2dx_allspace - normal end ==========================================
```





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   7b p2221b    66.6    526      40.5    396    -359.3   -53.8    0.00     0.00     19.4
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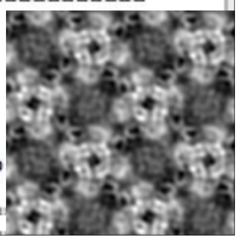
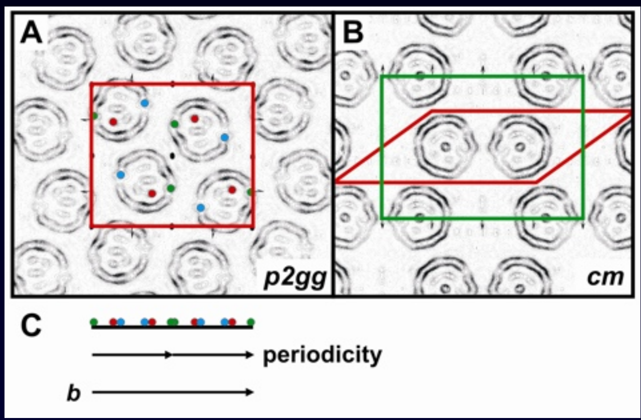
==== 2dx_allspace - normal end ==========================================
```

**Why 21 space groups?**



## Systematic absences

- *Symmetry forbidden reflections* result when a crystal has periodicity over less than one unit cell
- Axial/zonal systematic absences arise from glides/screws
  > Loss of odd reflections
- Integral systematic absences arise when a centered cell is chosen
  > Twice as many reflections

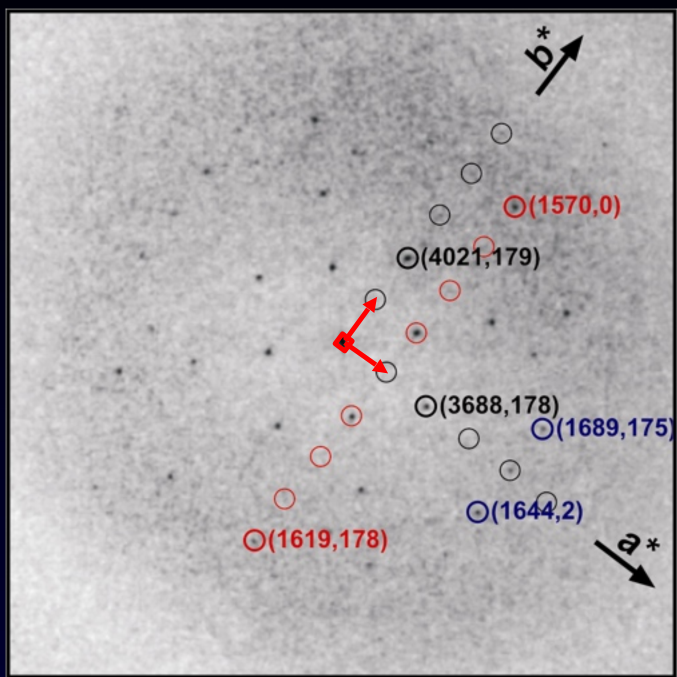



Slide by Michael Landsberg, Bribane, Australia



## Fourier space example – CHIP28 (Aqp1)

- *a=b, γ=90*
  - square unit cell
- all phases = 0/180
  - centrosymmetric space group
- points related by 4-fold rotation are equal
  - base symmetry is p4
- odd reflections absent
- spots equidistant from *a** are out of phase by 180
  - glide symmetry

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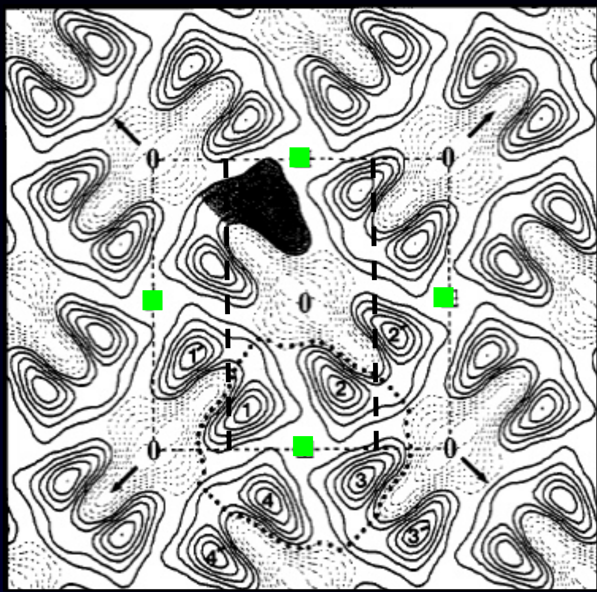
## CHIP28 (Aqp1) in real space

### *p4gm ($P42_12$)*

- 4 fold rotational symmetry
- 1 pair of glide axes
- 1 pair of mirror lines



Mitra et al. *Biochem* (1994) 33:12735-40

■ 4-fold center of rotation

- - - glide axis

⟶ mirror line

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## Other considerations

- When might symmetry fall apart?
  - Plane group symmetry rules only hold for untilted specimens
  - Astigmatism causes a non-uniform effect of the CTF on symmetry related spots, potentially making symmetry evaluation unreliable
  - Symmetry rules only hold when data are shifted to phase origin
  - Stain exclusion patterns can cause over-estimation of symmetry
  - Low resolution data may also over-estimate symmetry
- Always check for the satisfaction of sub-symmetries to help
- *ALLSPACE* does not check for systematic absences
- Check that symmetry rules continue to hold when merging and moving up in resolution

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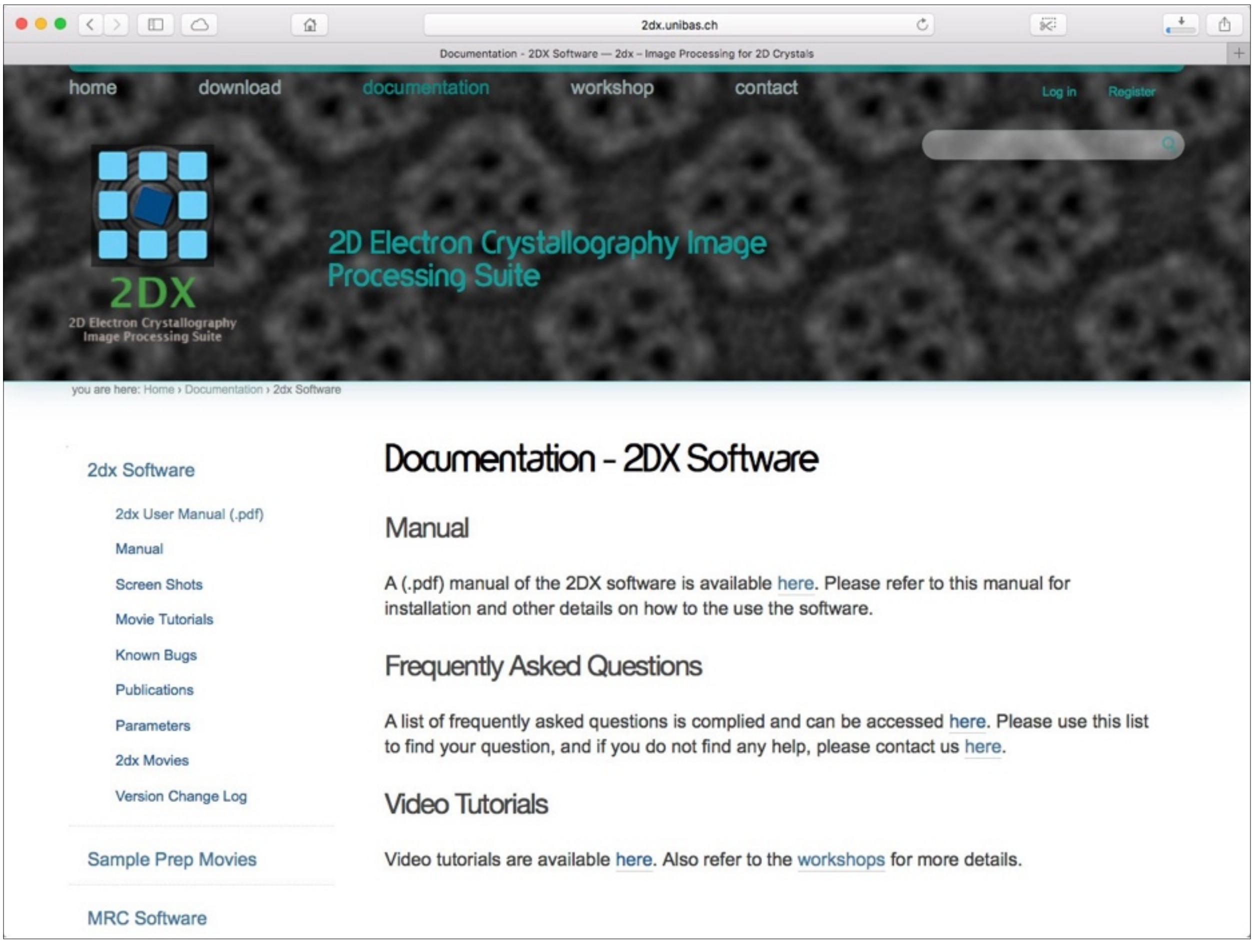
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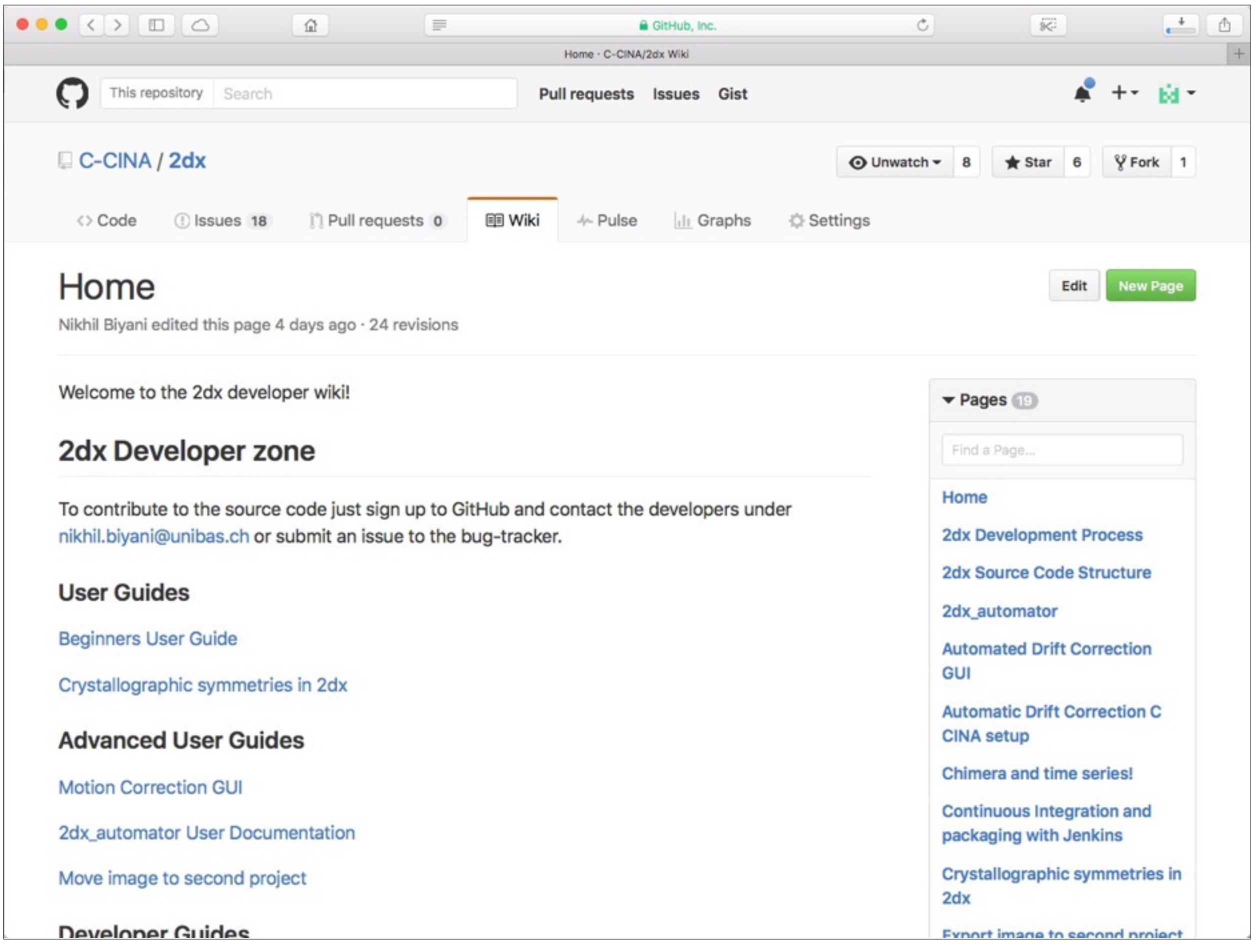
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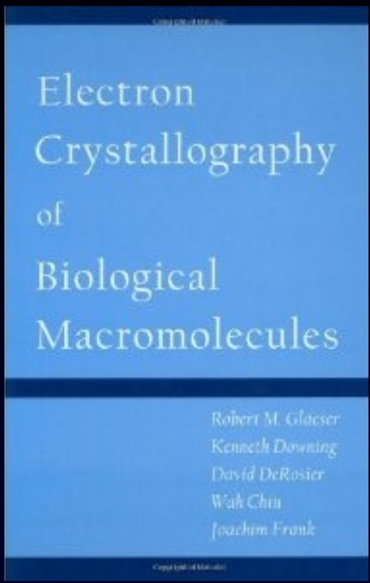
# Further Reading

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Symmetry: A guide to its application in 2D electron crystallography

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Received 1 May 2007; received in revised form 19 June 2007; accepted 6 July 2007
Available online 17 July 2007

…also: V. Unger *et al.* "Structure determination from electron micrographs of 2d crystals"

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