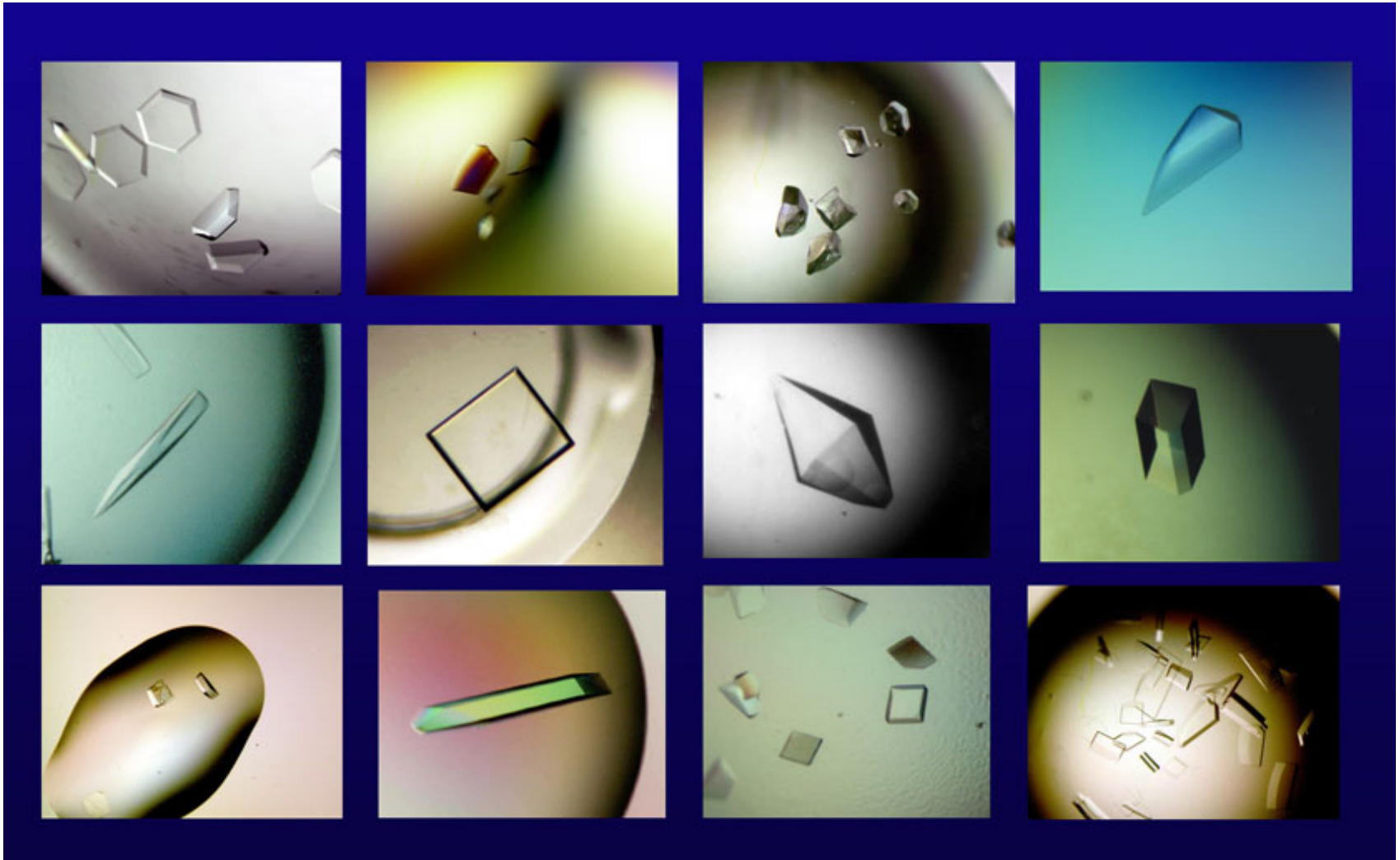
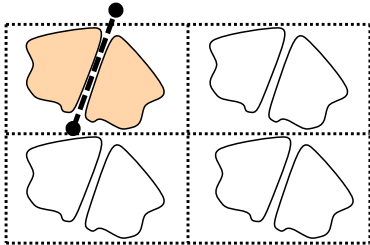


Introduction to crystal symmetry

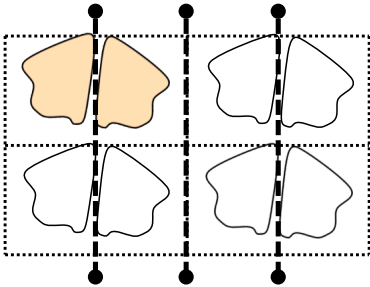
Andrey Lebedev, CCP4



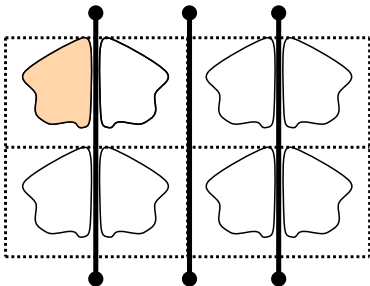
Symmetry, NCS and Pseudosymmetry



Generic Non-Crystallographic Symmetry (NCS):
- symmetry is **local** and **approximate**

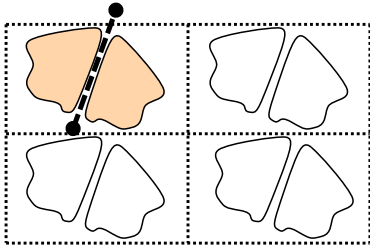


Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**

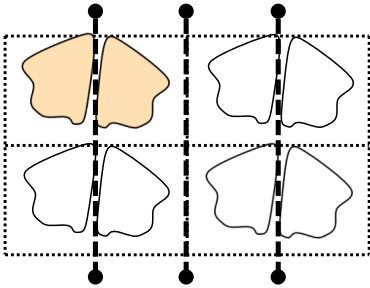


Crystallographic symmetry
- symmetry is **global** and **exact**

Symmetry, NCS and Pseudosymmetry

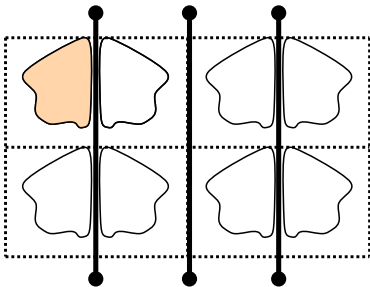


Generic Non-Crystallographic Symmetry (NCS):
- symmetry is **local** and **approximate**



Pseudosymmetry (a limiting case of NCS)
- symmetry is **global** and **approximate**

may be misinterpreted as crystallographic symmetry



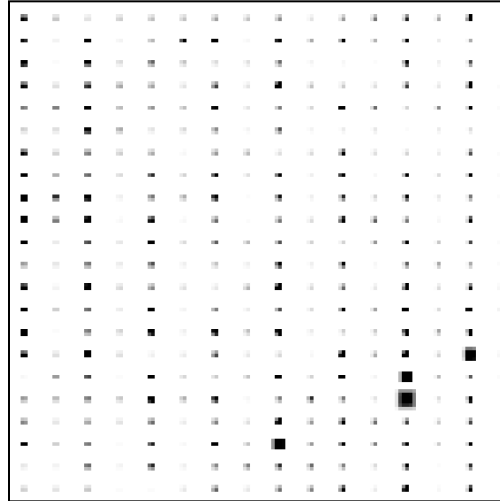
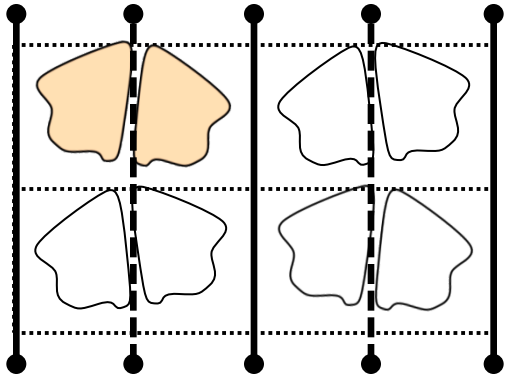
Crystallographic symmetry
- symmetry is **global** and **exact**

Pseudotranslation

Crystallographic translation



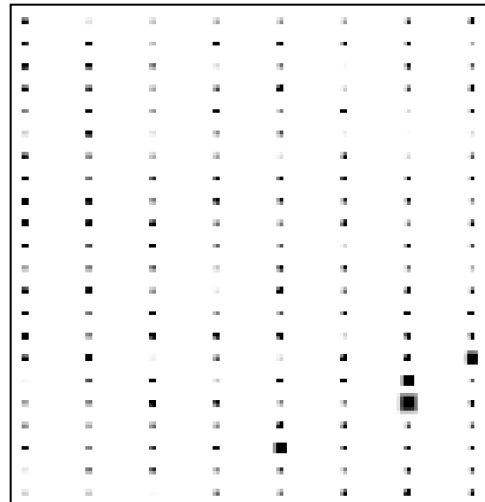
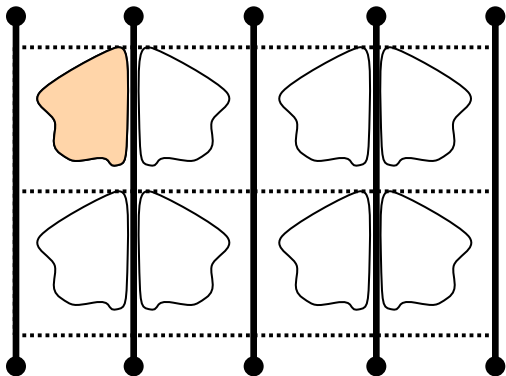
Pseudo-translation



Pseudotranslation $C/2$

Planes $2L+1$ contain weak reflections

Crystallographic translation



Limiting case, $C' = C/2$

- Weak reflections vanish

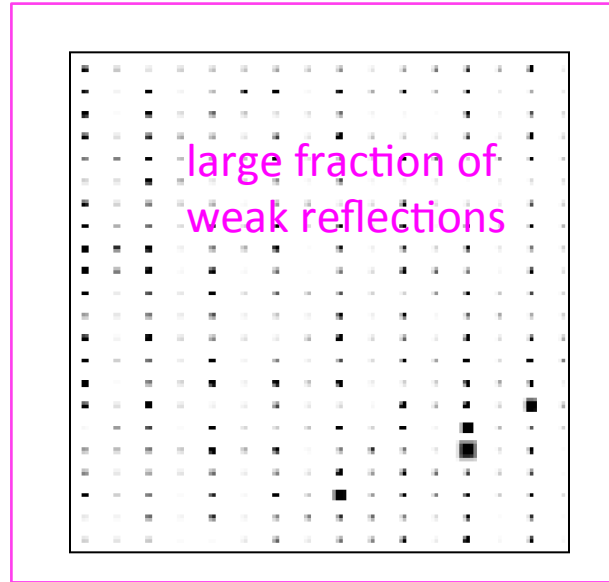
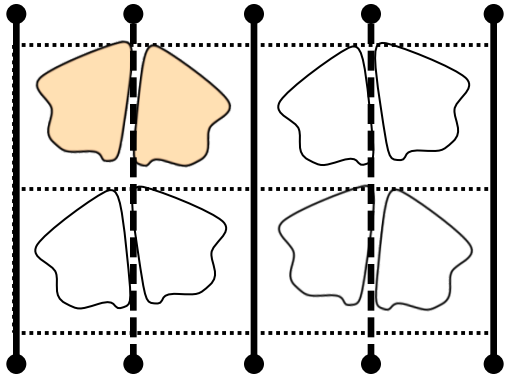
Two times larger
reciprocal lattice spacing

Pseudotranslation

Crystallographic translation



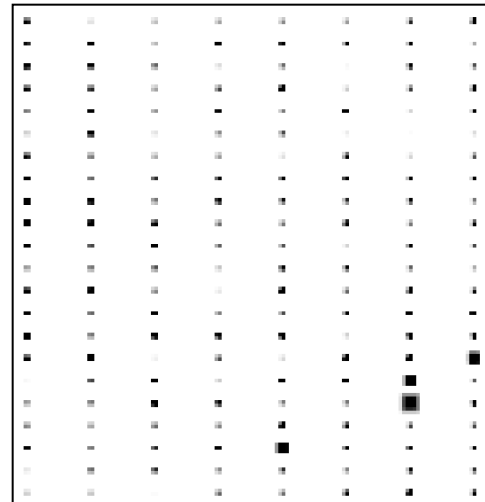
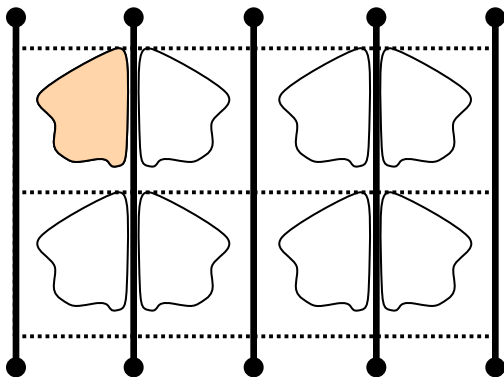
Pseudo-translation



Pseudotranslation $C/2$

Planes $2L+1$ contain weak reflections

Crystallographic translation



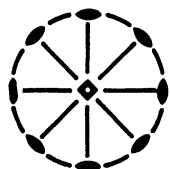
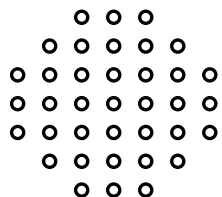
Limiting case, $C' = C/2$

- Weak reflections vanish

Two times larger
reciprocal lattice spacing

Space group assignment (*e.g. Pointless*)

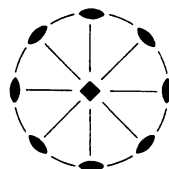
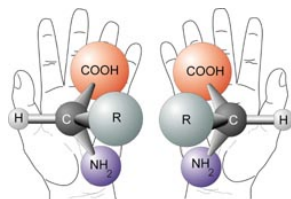
Reciprocal space lattice
(positions of reflections)



$4/m\bar{m}m$

Lattice
point group

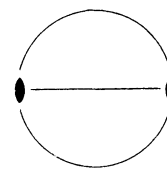
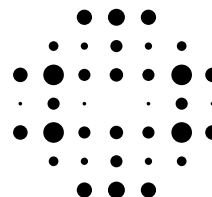
Mirror symmetry is not
allowed in biological
macromolecules



422

Highest possible
crystal point group

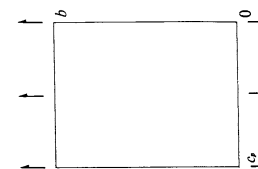
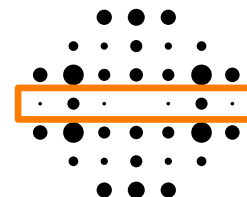
Intensities of
reflections



2

Probable
crystal point group

Intensities of axial
reflections



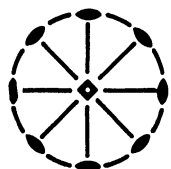
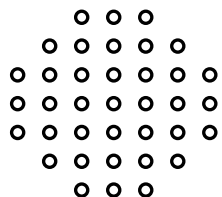
$P2_1$

Probable
crystal space group(s)

User: decision making

Space group assignment (*e.g. Pointless*)

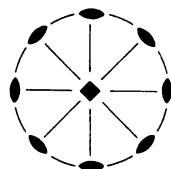
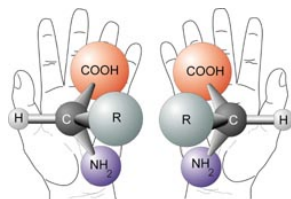
Reciprocal space lattice
(positions of reflections)



$4/mmm$

Lattice
point group

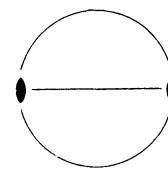
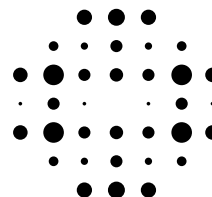
Mirror symmetry is not
allowed in biological
macromolecules



422

Highest possible
crystal point group

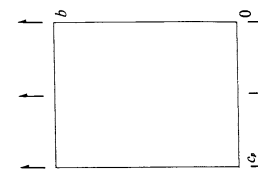
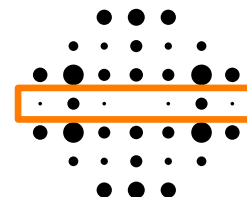
Intensities of
reflections



2

Probable
crystal point group

Intensities of axial
reflections

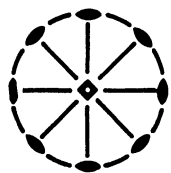


$P2_1$

Probable
crystal space group(s)

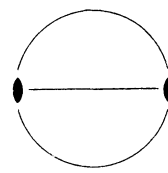


User: decision making



$4/mmm$

Lattice
point group



2

Probable
crystal point group

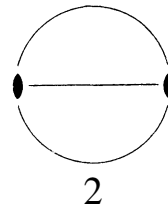
Online dictionary of Crystallography:

The point group of a crystal is called **merohedry** if it is a subgroup of the point group of its lattice.

In classification of twins, the word **pseudomerohedry** is used when the lattice has accidental high symmetry that is not defined by crystal symmetry (e.g. $\beta=90^\circ$ in $P\ 1\ 2_1\ 1$)



Lattice
point group

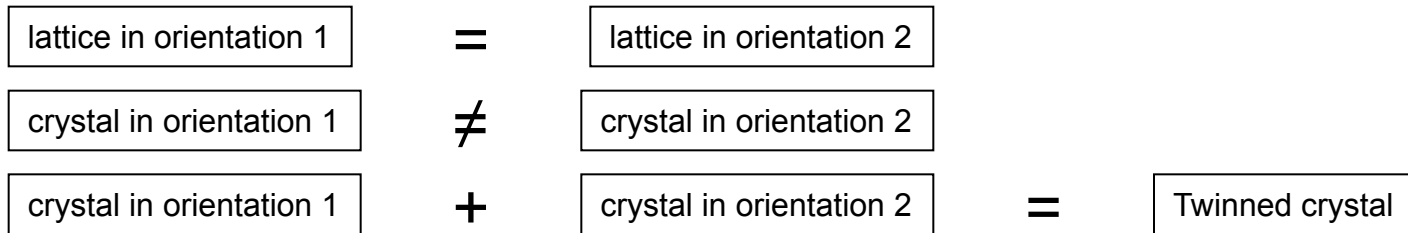


Probable
crystal point group

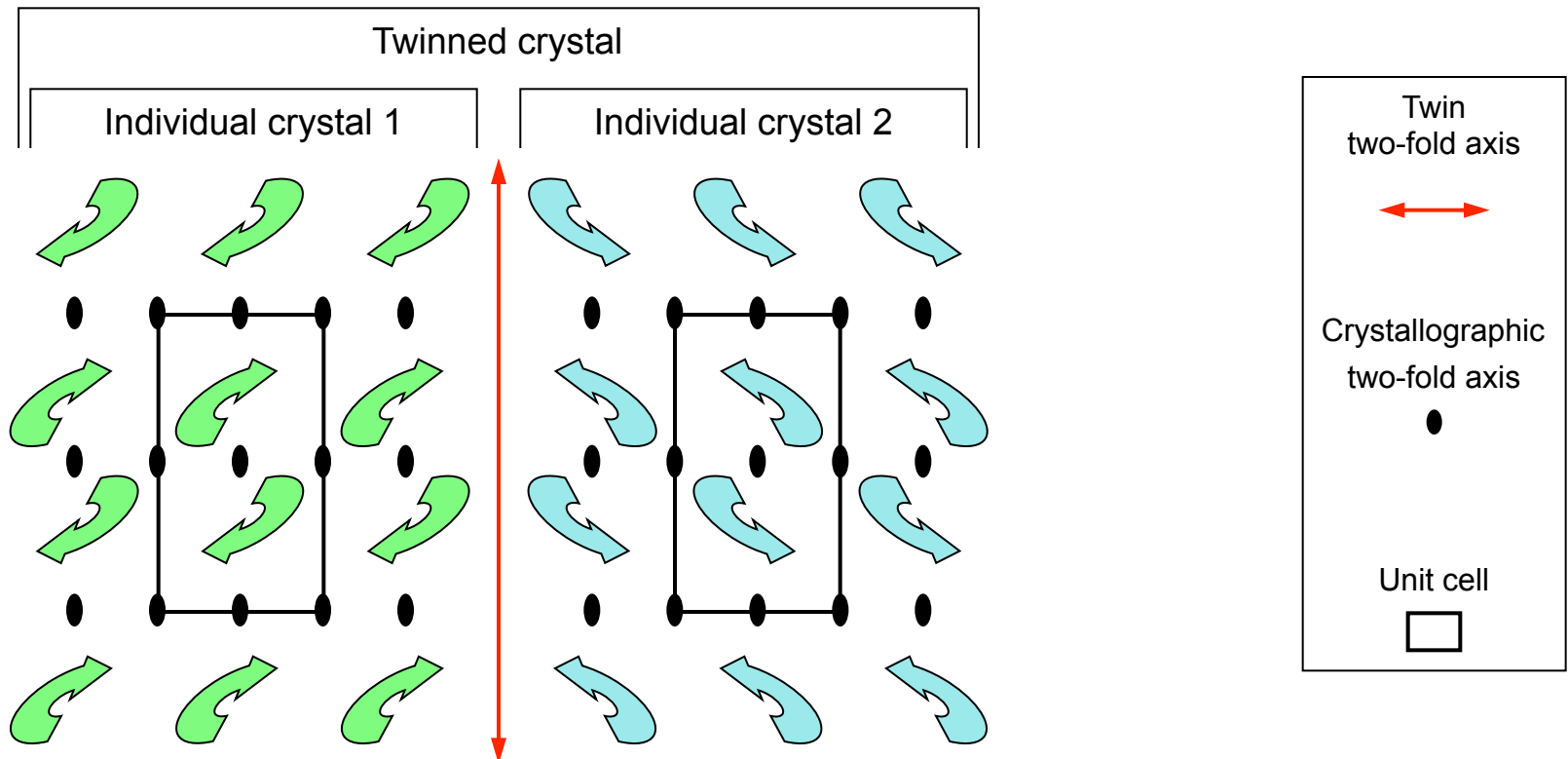
= **merohedry**

(Pseudo)merohedral twinning

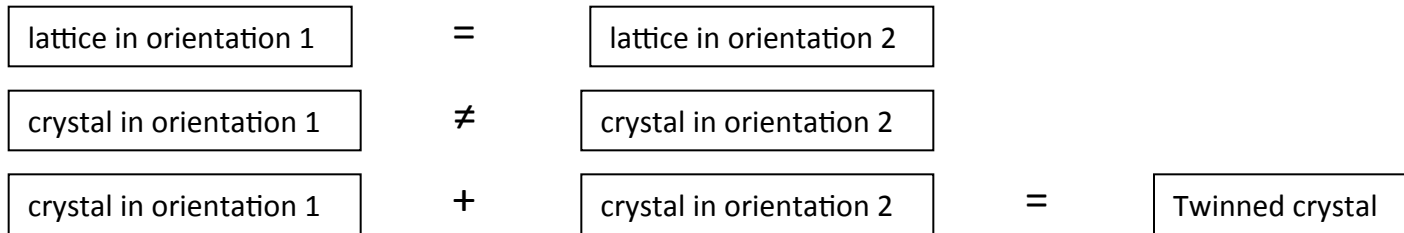
Twinning by (pseudo)merohedry



Example: P2, $\beta = 90$



Twinning by (pseudo)merohedry



P121, $\beta = 90$

Intensities from individual crystal 1

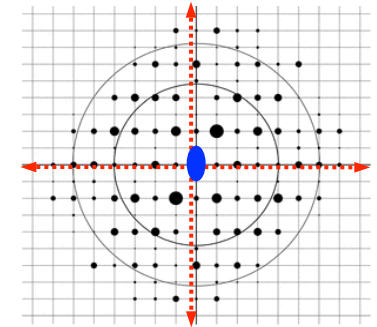
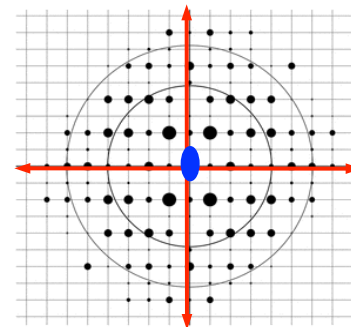
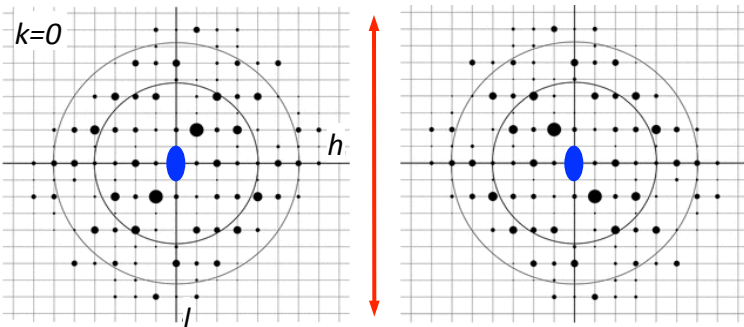
Intensities from individual crystal 2

Perfect twin

Partial twin

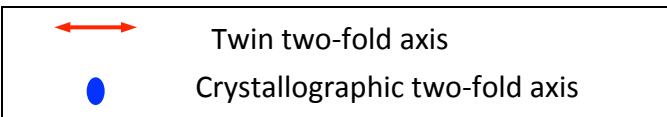
(individual crystals of equal sizes)

(individual crystals of different sizes)



less weak reflections

Allows for twinning tests based on statistics of intensities



Twinning tests

(Pseudo)merohedral twinning **cannot be readily seen** from diffraction images because reflections from twin individuals overlap:

- exactly in merohedral twins
- exactly or approximately in pseudomerohedral twins.

Weak reflections in "twinned data" are **less frequent** than "in non-twinned data".

This allows for twinning tests based on statistics of normalised intensities: cumulative distribution of normalised intensities, Britton test, second moments tests, H-test, L-test, ...

Twinning tests

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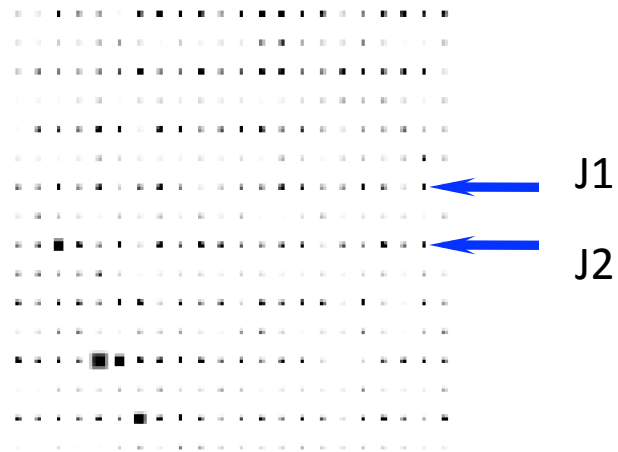
Weak reflections in "twinned data" are **less frequent** than "in non-twinned data".

This allows for twinning tests based on statistics of normalised intensities: cumulative distribution of normalised intensities, Britton test, second moments tests, H-test, L-test, ...

Pseudo-translation, if present, **increases** relative fraction of weak reflections and makes some of the twinning tests inconclusive.

L-test

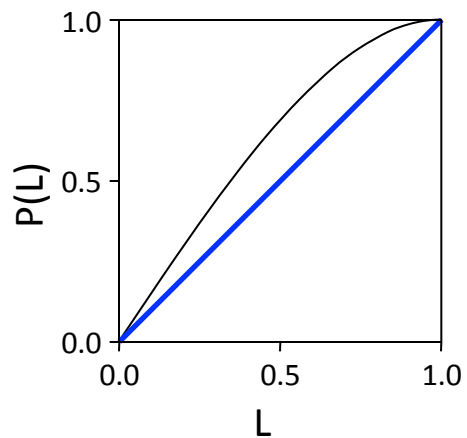
$$L = | J1 - J2 | / (J1 + J2)$$



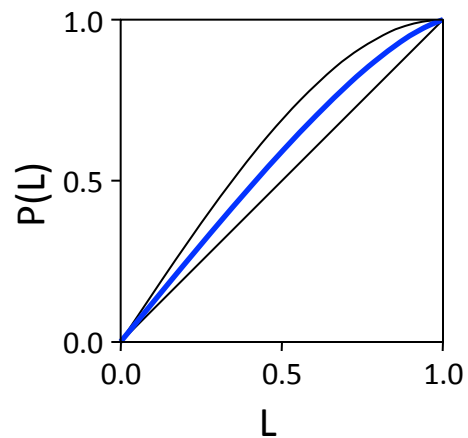
- L-test is designed to be suitable for most of cases
- with and without pseudo-translation
 - isotropic and anisotropic data

Theoretical distribution of L

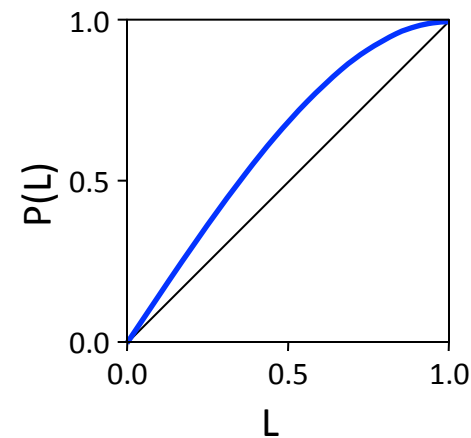
Single crystal



Partial twin



Perfect twin



CCP4i

Aimless

CCP4Interface 7.0.026 running on rccp4ws033.rc-harwell.ac.uk Project: exp3

List of jobs for project. Double-click on a job displays the log file, shift-double-click reruns the job.

Job ID	Time	Status	Program	Notes
6	11:44:29	FINISHED	aimless	[N]
1	11:22:27	FINISHED	aimless	[N]

Directories&ProjectDir

View Any File

View Files from Job

qtRView 1.16 - Job 6: [No title given]

Print PDF/PS Refresh aimless CCP4

Symmetry, Scale, Merge (Aimless)

Find Symmetry, Scale & Merge (Scala)

Multiple dataset analysis (Blend)

Utilities

Check Data Quality

L-test for twinning
(no twinning)

Job 6: [No title given]

- Analysis against resolution, with & without anomalous (Ov), XDSdataset
- Analysis against intensity, XDSdataset
- Completeness & multiplicity v. resolution, XDSdataset
- Run 1, standard deviation v. Intensity, XDSdataset
- Radiation damage analysis for run 1
- Effect of parameter variance on sd(l)

Run of truncate on 17/12/2016 at 11:44:22

Graph Data

- Intensity Completeness analysis
- Wilson plot
- Intensity anomalous analysis
- Intensity statistics
- Cumulative intensity distribution
 - L test for twinning
 - cumulative distribution function for |L|, twin f...
 - Untwinned
 - Twinned
- Acentric Moments of I
- Centric Moments of I
- H test for twinning
- Britton plot for twinning
- ML-Britton test for twinning
- Phil plot

mulative distribution function for |L|, twin fraction of 0

Data reduction - AIMLESS

CCP4-7.0.065 Project Viewer: xia2

Task menu Export project Run Run on server Clone job Help Bibliography Export MTZ Show log file

Job list Project directory

Filter: Only show jobs containing text typed here

Filter: Only show jobs containing text typed here

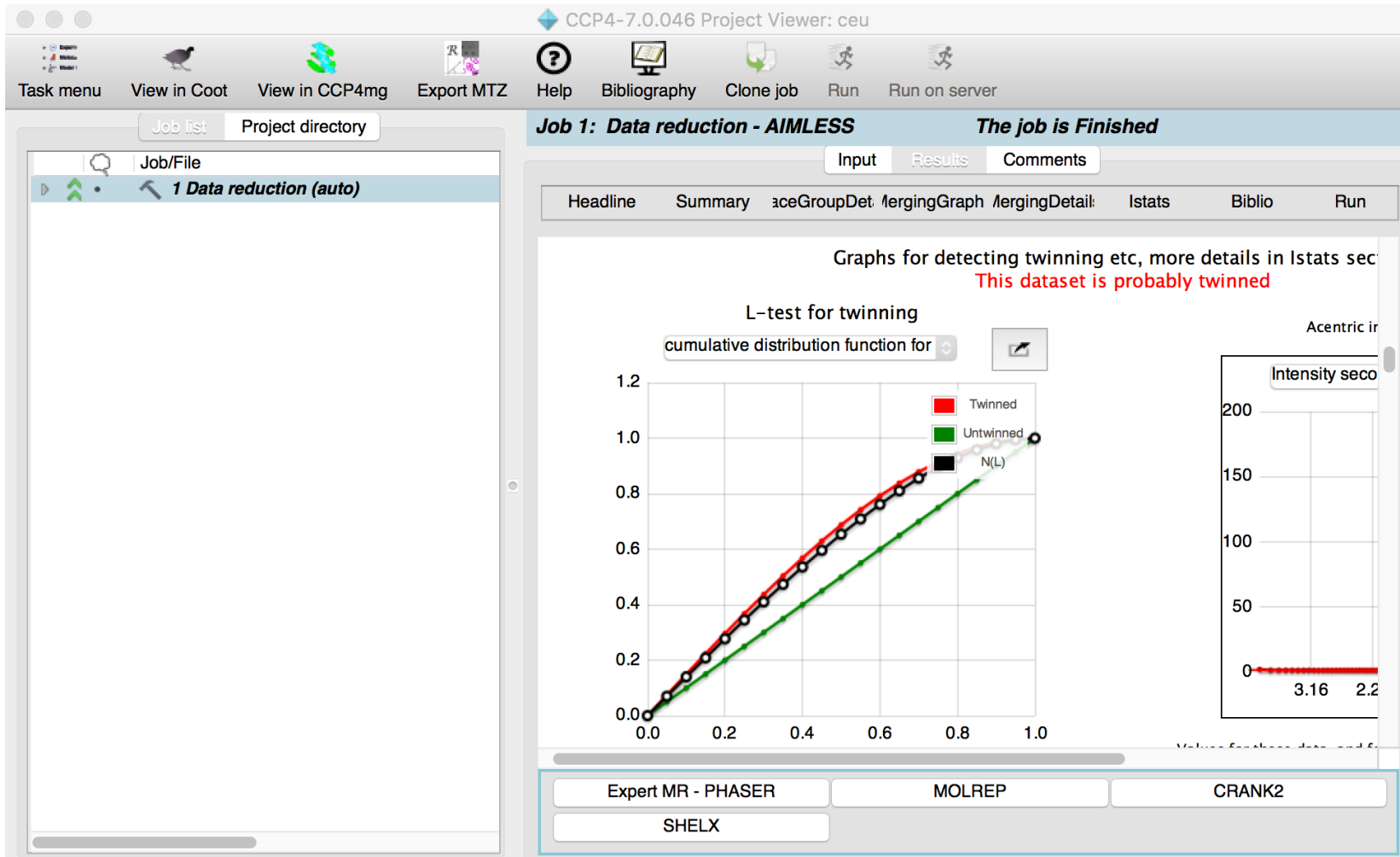
Job/File E
 ▶ 3 Data reduction S
 ▶ 2 xia2/dials S
 ▶ 1 xia2/dials S

Filter: Only show tasks containing text typed here

- ▶ Import merged data, crystal contents, alignments or coordinates
- ▶ Integrate X-ray images
- ▼ X-ray data reduction and analysis
 - Data reduction - AIMLESS**
Scale and analyse unmerged data and suggest space group (Pointless, Aimless, Ctruncate, FreeRflag)
 - Generate a Free R set**
Generate a Free R set for a complete set of reflection indices to a given resolution (FreeRflag)
 - Estimate cell content**
Estimate number of molecules in the asymmetric unit and solvent content (Matthews_coeff)
 - Calculate self rotation function**
Evaluate data for anisotropy, optical resolution, pseudo translation and perform self-rotation function (Molrep)
 - Graphical diagnostics by AUSPEX plots**
Use AUSPEX, generate graphical diagnostics for data set
- ▶ Experimental phasing
- ▶ Bioinformatics including model preparation for Molecular Replacement
- ▶ Molecular Replacement
- ▶ Density modification
- ▶ Model building and Graphics
- ▶ Refinement

New job Cancel

L-test plot and also a warning on possible twinning



Scores for each symmetry element

CCP4-7.0.065 Project Viewer: xia2

Task menu Export project Run Run on server Clone job Help Bibliography Export MTZ Show log file

Job list Project directory

Filter: Only show jobs containing text typed here

- 3 Data reduction
- 2 xia2/dials
- 1 xia2/dials

Job 3: Data reduction - AIMLESS **The job is Finished**

Input Results Comments

Headline Summary SG details MergingGraphs SDanalysis MergingDetails Istats Biblio Run

▼ Overall summary

Space group determination

Selecting point group P 2 2 2
as multiple space groups have the same score

WARNING: You will have to determine the true space group later
The 'space group' written to output file may be missing possible screw components

Solution type: point group

Group name	P 2 2 2
Reindex	[h,k,l]
Space group confidence	0.000
Laue group confidence	0.992
Laue group probability	0.002
Systematic absence probability	0.751

Scores for each symmetry element

Lattice group name P 2 2 2

Likelihood	CC	R		Symmetry
0.942	0.97	0.117		identity
0.955	0.98	0.081	***	2-fold l (0 0 1) {-h,-k,l}
0.954	0.98	0.095	***	2-fold k (0 1 0) {-h,k,-l}
0.954	0.98	0.095	***	2-fold h (1 0 0) {h,-k,-l}

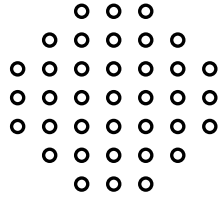
Data internal consistency statistics

Summary of merging statistics for dataset xia2/a/b

	Overall	Inner	Outer
Low resolution limit	32.63	32.63	1.73
High resolution limit	1.69	8.96	1.69
Rmerge(within I+ /I-)*	0.066	0.038	0.000
Rmerge(all I+ and I-)*	0.086	0.056	0.000
Rmeas (within I+ /I-)*	0.091	0.054	0.000
Rmeas (all I+ & I-)*	0.115	0.074	0.000
Rpim (within I+ /I-)	0.062	0.038	0.000
Rpim (all I+ & I-)	0.076	0.048	0.000
Rmerge in top intensity bin*	0.042		
Number of observations	13126	162	14
Number unique	9175	98	14

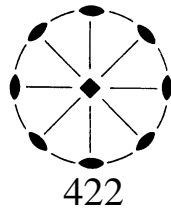
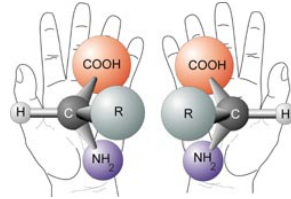
Space group assignment (*e.g. Pointless*)

Reciprocal space lattice
(positions of reflections)



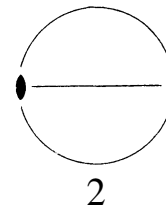
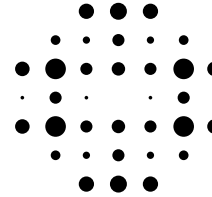
Lattice
point group

Mirror symmetry is not
allowed in biological
macromolecules



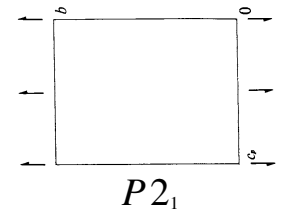
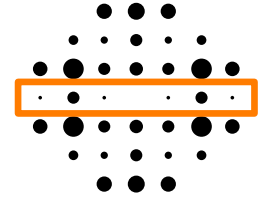
Highest possible
crystal point group

Intensities of
reflections



Probable
crystal point group

Intensities of axial
reflections



Probable
crystal space group(s)



User: decision making

Untwinned data

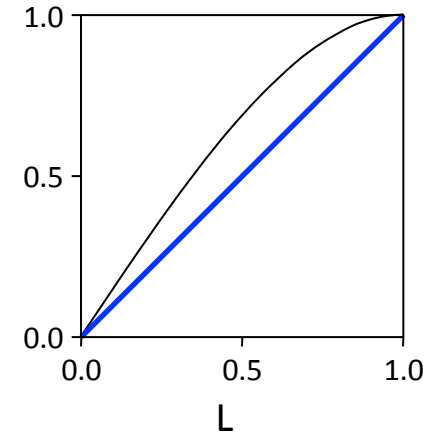
Scores for each symmetry element

Lattice group name P 6 2 2

Reindex operator from input to lattice: [h,k,l]

Likelihood	CC	R		Symmetry
0.952	0.97	0.146		identity
0.954	0.98	0.111	***	2-fold l (0 0 1) {-h,-k,l}
0.956	0.99	0.075	***	2-fold k (0 1 0) {-h,h+k,-l}
0.955	0.98	0.098	***	2-fold h (1 0 0) {h+k,-k,-l}
0.954	0.98	0.128	***	2-fold (1-1 0) {-k,-h,-l}
0.954	0.98	0.112	***	2-fold (2-1 0) {h,-h-k,-l}
0.956	0.99	0.100	***	2-fold (-1 2 0) {-h-k,k,-l}
0.954	0.98	0.119	***	2-fold (1 1 0) {k,h,-l}
0.953	0.97	0.105	***	3-fold l (0 0 1) {k,-h-k,l}
0.954	0.98	0.112	***	6-fold l (0 0 1) {h+k,-h,l}

Single crystal



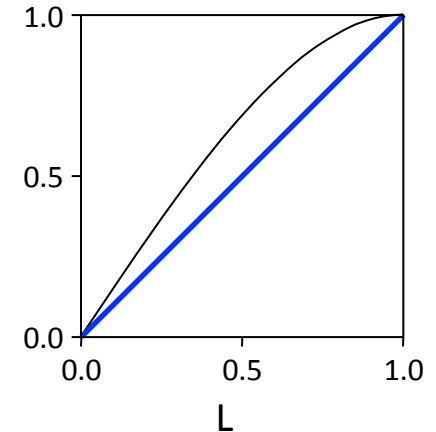
This is a **single** crystal, **P622** or **P6₁22** or **P6₂22** or ...

Pseudosymmetry

Scores for each symmetry element
Lattice group name P 6 2 2
Reindex operator from input to lattice: [h,k,l]

Likelihood	CC	R		Symmetry
0.898	0.90	0.060		identity
0.079	0.23	0.678		2-fold l (0 0 1) {-h,-k,l}
0.778	0.75	0.169	**	2-fold k (0 1 0) {-h,h+k,-l}
0.819	0.77	0.163	**	2-fold h (1 0 0) {h+k,-k,-l}
0.824	0.77	0.163	**	2-fold (1 -1 0) {-k,-h,-l}
0.077	0.22	0.675		2-fold (2 -1 0) {h,-h-k,-l}
0.079	0.22	0.674		2-fold (-1 2 0) {-h-k,k,-l}
0.080	0.23	0.675		2-fold (1 1 0) {k,h,-l}
0.903	0.88	0.089	***	3-fold l (0 0 1) {k,-h-k,l}
0.078	0.22	0.619		6-fold l (0 0 1) {h+k,-h,l}

Single crystal



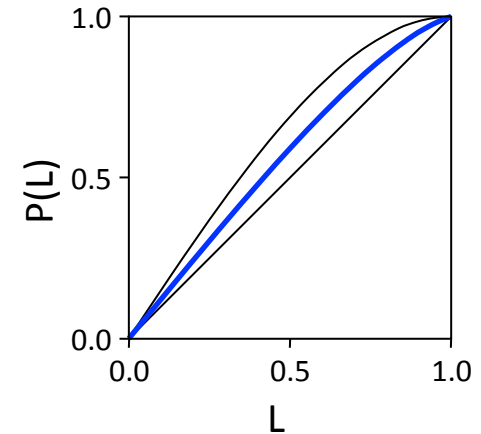
This is a **single** crystal, **P3** or **P3₁** or **P3₂**
There is a pseudosymmetry

Partial twin

Scores for each symmetry element
Lattice group name P 6 2 2
Reindex operator from input to lattice: [h,k,l]

Likelihood	CC	R		Symmetry
0.898	0.90	0.060		identity
0.079	0.23	0.678		2-fold l (0 0 1) {-h,-k,l}
0.778	0.75	0.169	**	2-fold k (0 1 0) {-h,h+k,-l}
0.819	0.77	0.163	**	2-fold h (1 0 0) {h+k,-k,-l}
0.824	0.77	0.163	**	2-fold (1 -1 0) {-k,-h,-l}
0.077	0.22	0.675		2-fold (2 -1 0) {h,-h-k,-l}
0.079	0.22	0.674		2-fold (-1 2 0) {-h-k,k,-l}
0.080	0.23	0.675		2-fold (1 1 0) {k,h,-l}
0.903	0.88	0.089	***	3-fold l (0 0 1) {k,-h-k,l}
0.078	0.22	0.619		6-fold l (0 0 1) {h+k,-h,l}

Partial twin



This is a **partial twin**, P3 or P3₁ or P3₂
There may be a pseudosymmetry

Perfect twin

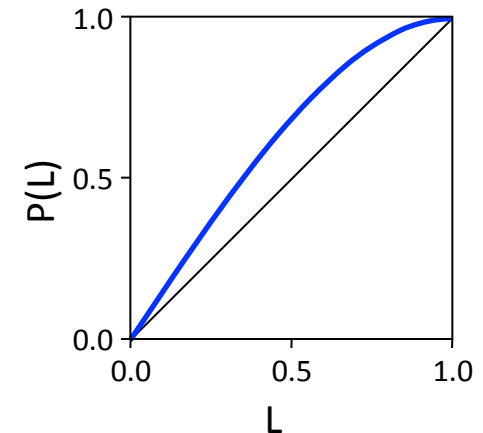
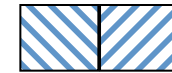
Scores for each symmetry element

Lattice group name P 6 2 2

Reindex operator from input to lattice: [h,k,l]

Likelihood	CC	R		Symmetry
0.952	0.97	0.146		identity
0.954	0.98	0.111	***	2-fold l (0 0 1) {-h,-k,l}
0.956	0.99	0.075	***	2-fold k (0 1 0) {-h,h+k,-l}
0.955	0.98	0.098	***	2-fold h (1 0 0) {h+k,-k,-l}
0.954	0.98	0.128	***	2-fold (1-1 0) {-k,-h,-l}
0.954	0.98	0.112	***	2-fold (2-1 0) {h,-h-k,-l}
0.956	0.99	0.100	***	2-fold (-1 2 0) {-h-k,k,-l}
0.954	0.98	0.119	***	2-fold (1 1 0) {k,h,-l}
0.953	0.97	0.105	***	3-fold l (0 0 1) {k,-h-k,l}
0.954	0.98	0.112	***	6-fold l (0 0 1) {h+k,-h,l}

Perfect twin



This is likely to be a **perfectly twinned crystal**.

Space group is quite uncertain at this point.

Most likely:

the space group is **NOT** $P6_x22$

but one of its subgroups:

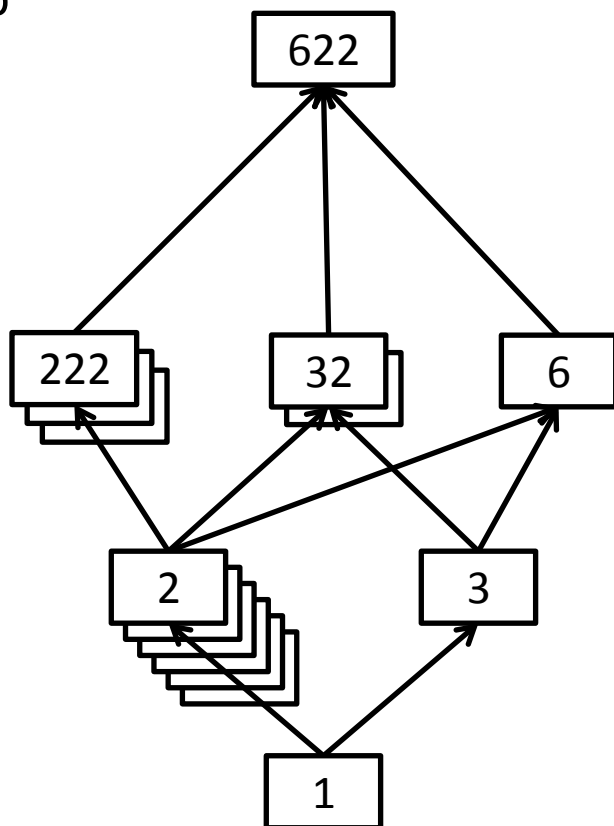
$P6_x$, $P3_x21$, $P3_x12$, $C222_x$, or even $P3$ etc.

Subgroups of the point group 622

supergroup



subgroup



- To test all possibilities, we have to run Phaser once for each point group and ask to try all the corresponding space groups
- E.g. for point group 3, Phaser will try P 3, P 3₁, P3₂.

An alternative approach: structure solution in P1

Can be used with close homologues and requires complete data in P1

- Scale and merge data in P 1 (Aimless)
- Solve in P1
- Use Zanuda program to restore the correct space group

Forcing P 1 space group assignment

CCP4-7.0.046 Project Viewer: ceu

Task menu View in Coot View in CCP4mg Export MTZ Help Bibliography Clone job Run Run on server

Job list Project directory

Job/File

- 2 Data reduction
- 1 Data reduction

Job 2: Data reduction - AIMLESS *The job is Pending*

Input Results Comments

Input Data Important Options Additional Options

Job title Data reduction

Use data from job No as input below..

Show list Select unmerged data files

1 Unmerged reflections loaded from mx1221v56_ceueb1HA00AR19284_SAD_

Crystal name ceu dataset name ceu

Batches in file:

Exclude batches from calculations and output

Resolution range (A) to 1.6 Maximum resolution in files 0.00Å

use explicit resolution range in symmetry determination as well as in scaling

Options for symmetry determination Choose a known or previous solution

Options for choice of space group or Laue group:

Perform search then choose spacegroup P 1

Reindex operator h= h k= k l= l

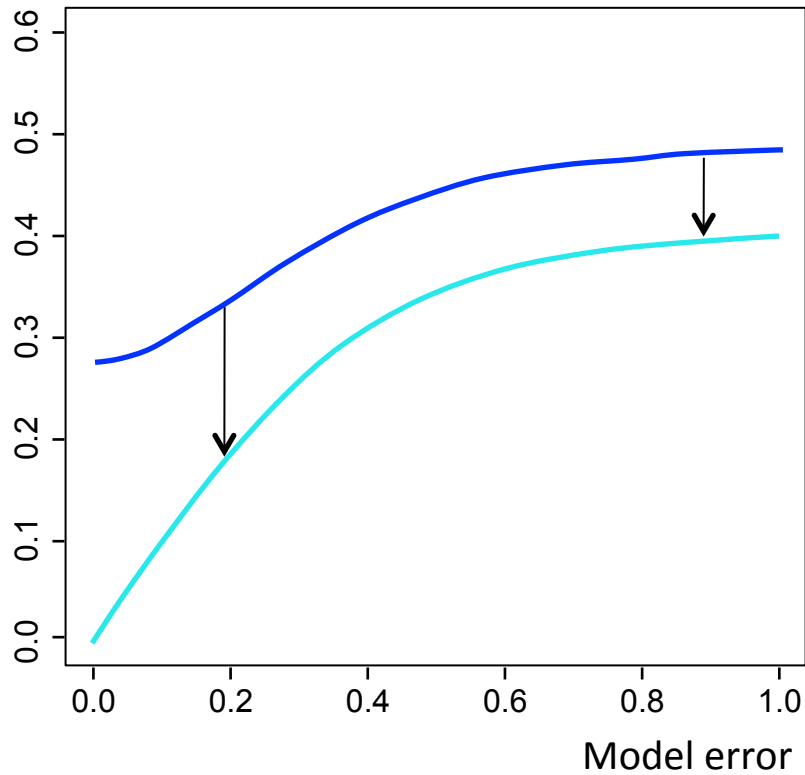
Optional input data

Switching to twin refinement

Twin refinement: Off On

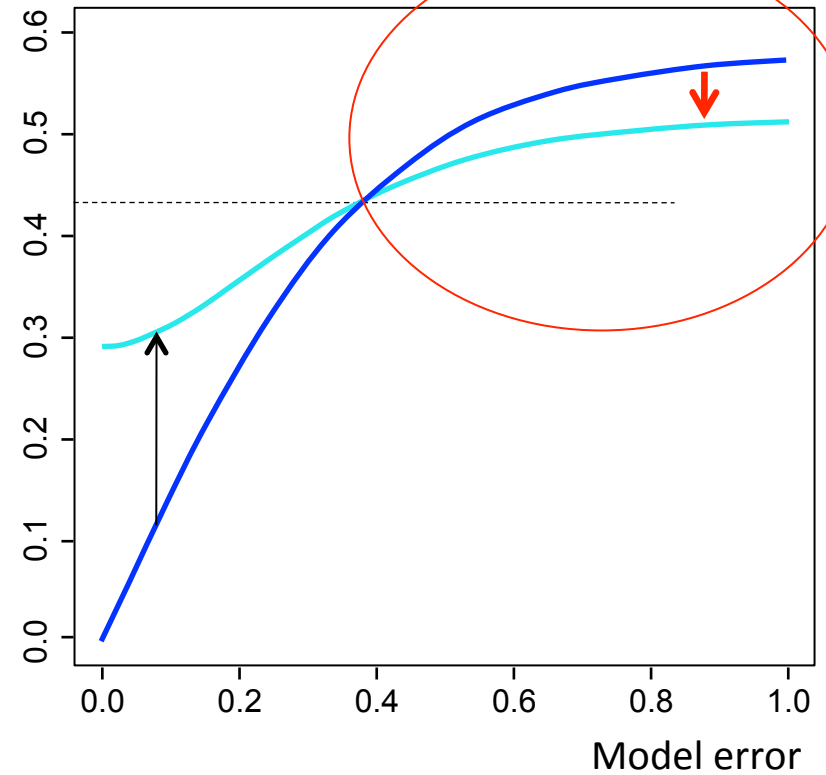
Twinned crystal

R-factor



Single crystal

R-factor



End