Data problems:

How to spot them and what to do

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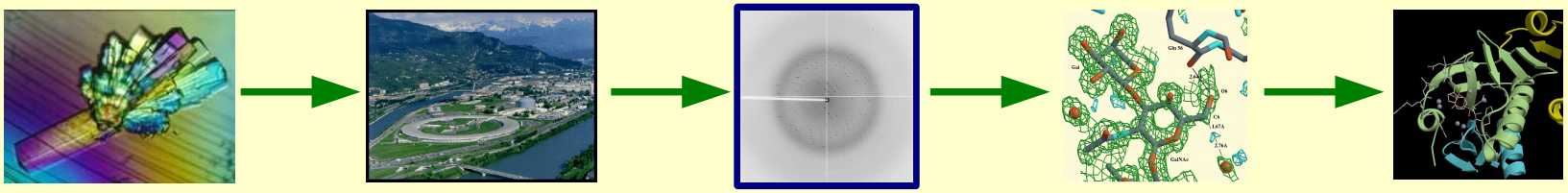
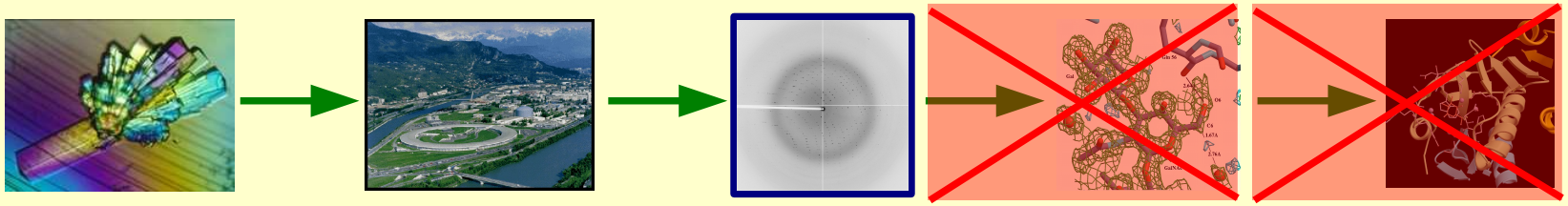
CCP4 Study Weekend 2010
Nottingham, UK

Introduction



nice linear path from crystal to final structure

Introduction

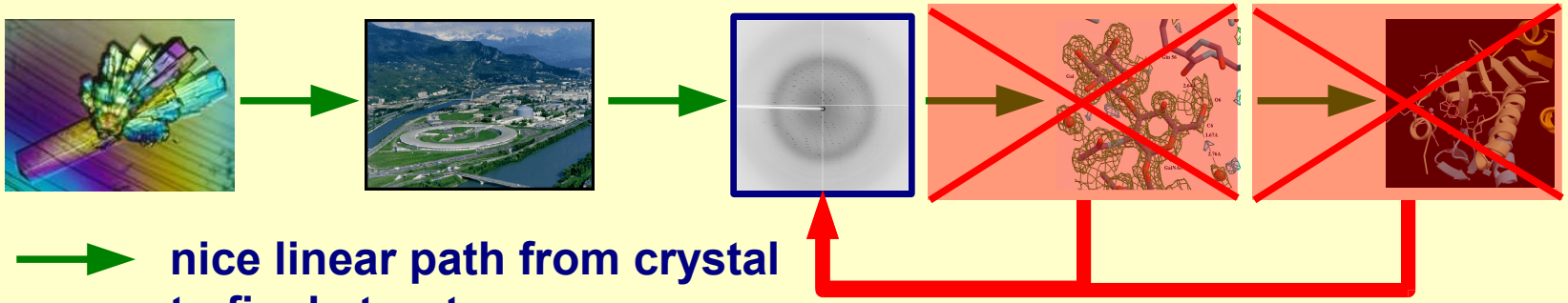


nice linear path from crystal to final structure

- problematic refinement
- Rfree 'stuck'
- unclear density
- disordered domain not visible

- no heavy atom substructure
- poor phasing power
- spacegroup uncertain
- density too poor to build into

Introduction



→ nice linear path from crystal to final structure

Problems with:

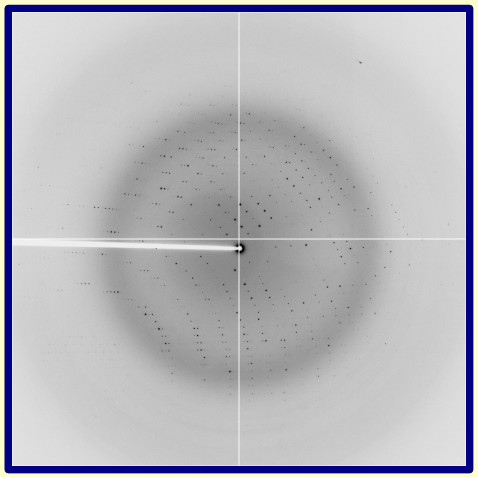
- Crystal form
- Crystal handling
- Collection strategy
- Data processing
- Data characteristics

→ distinguish features we have no immediate control over from problems we can deal with

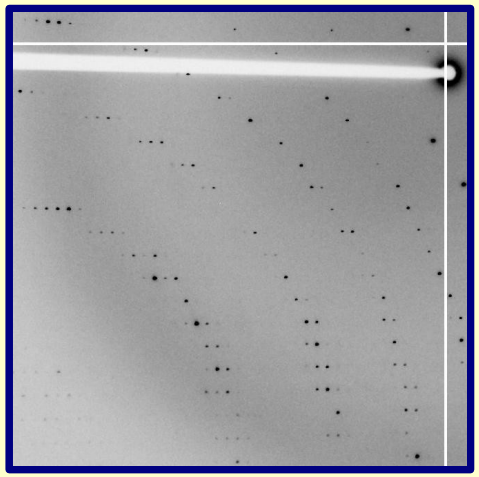
- problematic refinement
- Rfree 'stuck'
- unclear density
- disordered domain not visible

- no heavy atom substructure
- poor phasing power
- spacegroup uncertain
- density too poor to build into

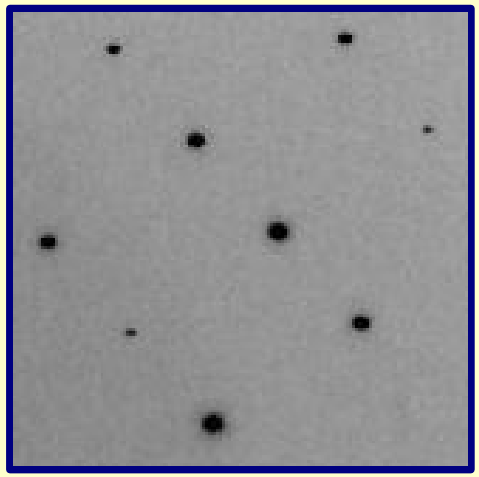
Expectations



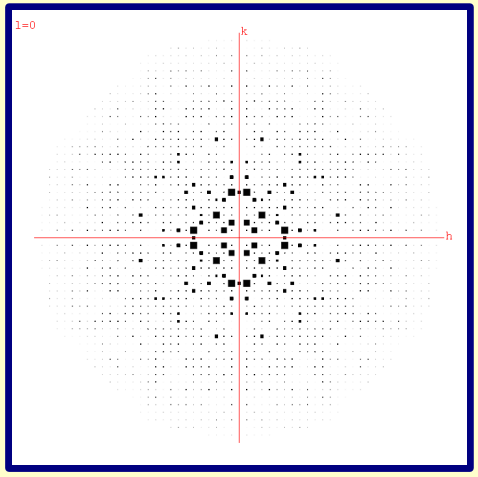
nice diffraction



separated lunes



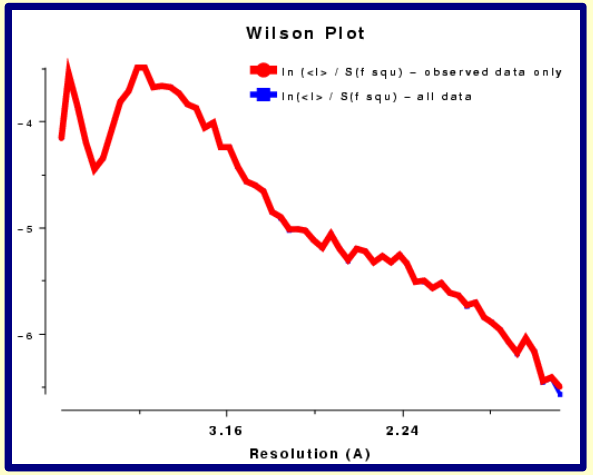
perfect spots



completeness

ideal world

well behaved statistics



How it usually starts ...

From: XYZ
Subject: Need help!
To: vonrhein@GlobalPhasing.com
Date: Thu, 31 Feb 2009 12:28:22

Dear Clemens,

I've collected several datasets but can't solve my structure. What should I do?

Kind regards

XYZ

From: [redacted]
Subject: Help sought for problem dataset
To: vonrhein@GlobalPhasing.com
Date: [redacted]

Hi Clemens,

My problem is that my Rfree is down at 38% and I can't get it to drop any further. The data are very anisotropic and the maps from solomon look like 4A maps (the data go to 2.4A).

Any advice would be appreciated.

Thanks,

[redacted]

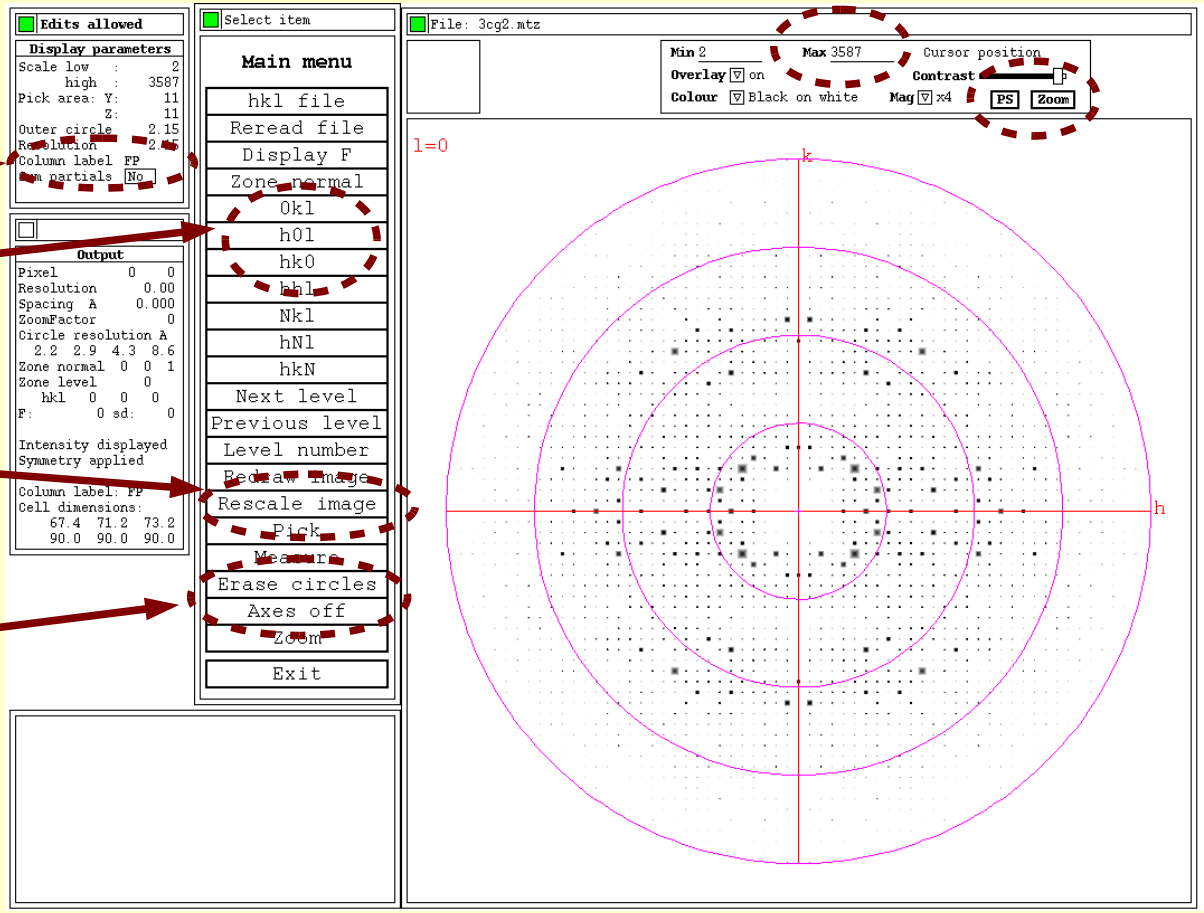
Take a step back to gather evidence

- Bring in the usual suspects

- Tie up loose ends

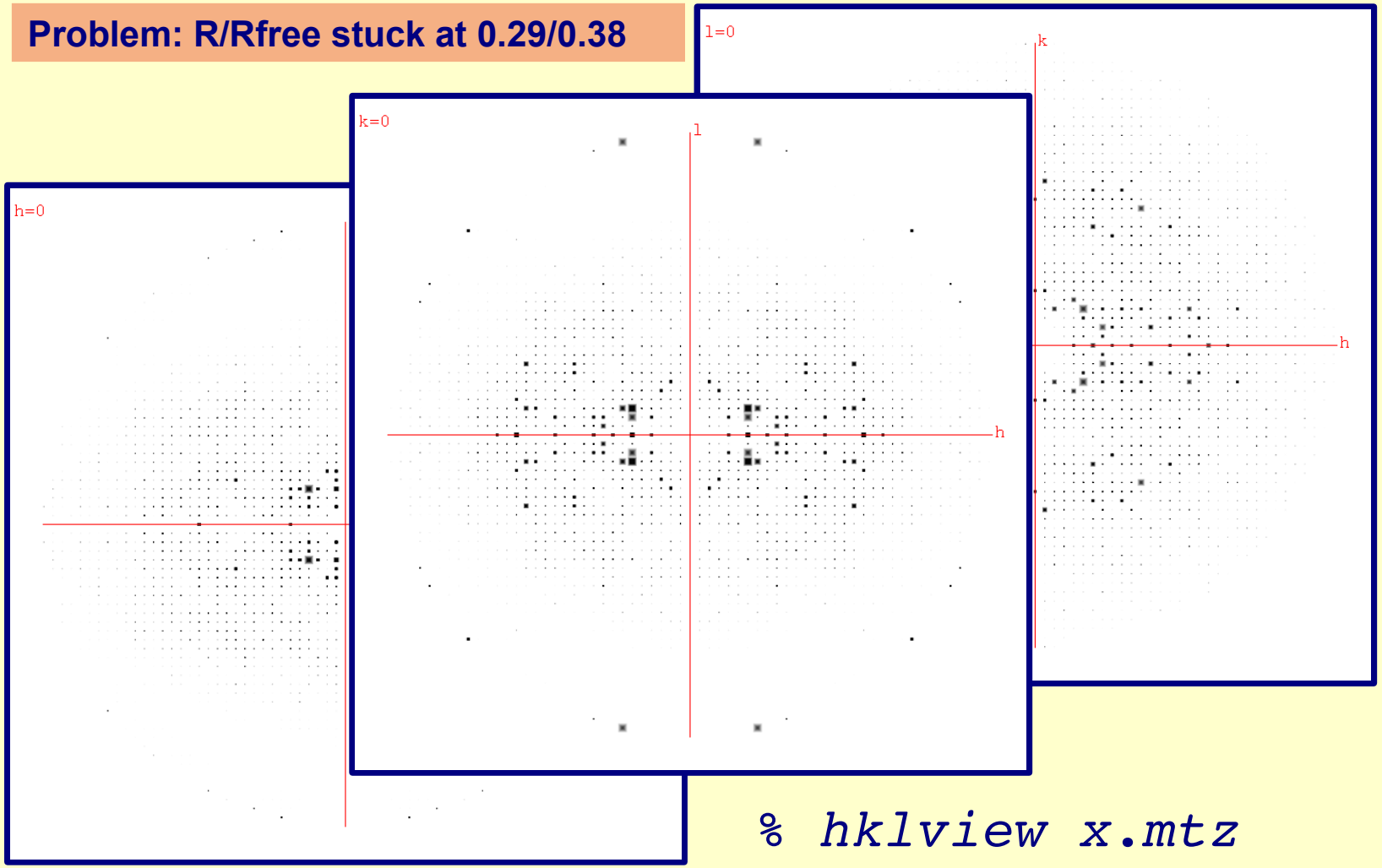
Looking at diffraction data - 1

hklview (P. Evans, xdl_view library by J. Campbell)
not (yet?) in ccp4i



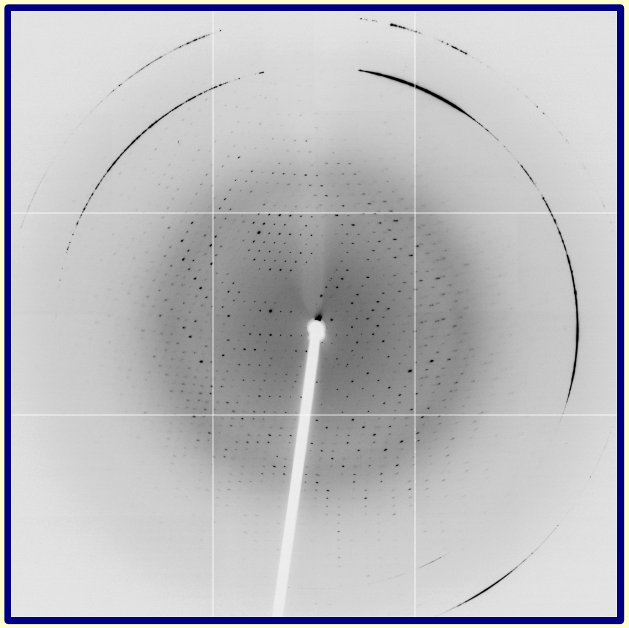
Looking at diffraction data - 2

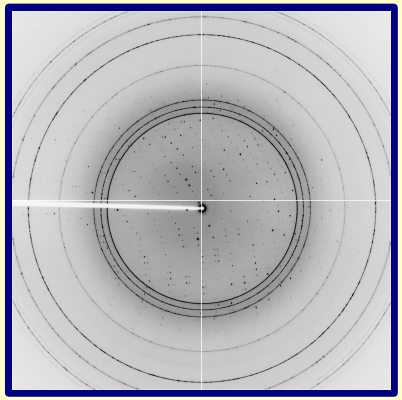
Problem: R/Rfree stuck at 0.29/0.38

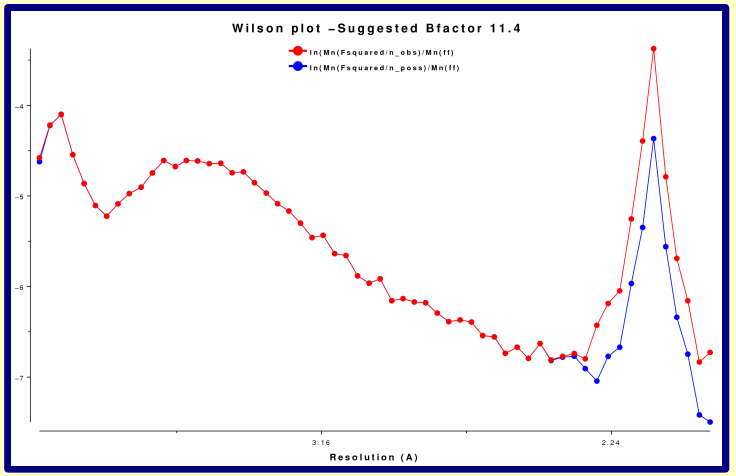



```
% hklview x.mtz
```

Ice-rings - 1

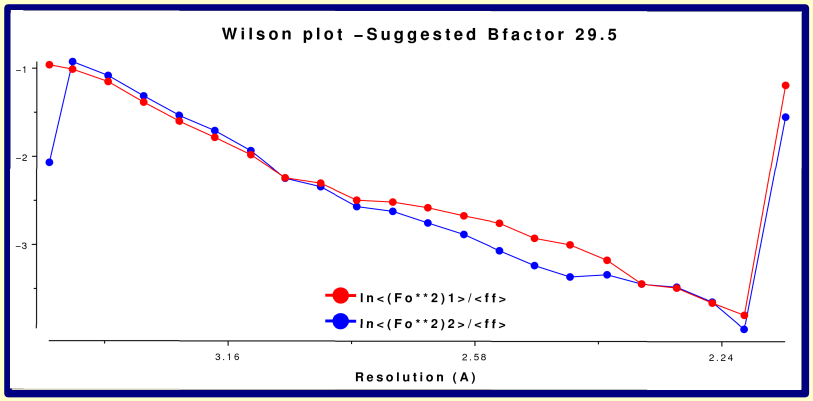






	Overall	InnerShell	OuterShell
Low resolution limit	73.39	73.39	2.17
High resolution limit	2.06	6.50	2.06
Rmerge	0.076	0.036	0.367
Ranom	0.046	0.010	0.476
Rmeas (within I+/I-)	0.089	0.042	0.514
Rmeas (all I+ & I-)	0.093	0.040	0.634
Rpim (within I+/I-)	0.089	0.021	0.360
Rpim (all I+ & I-)	0.093	0.015	0.421
Total number of observations	120693	5371	2465
Total number unique	19609	809	1589
Mean(I)/sd(I)	15.6	34.4	2.3
Completeness	86.6	99.6	49.3
Multiplicity	6.2	6.6	1.6

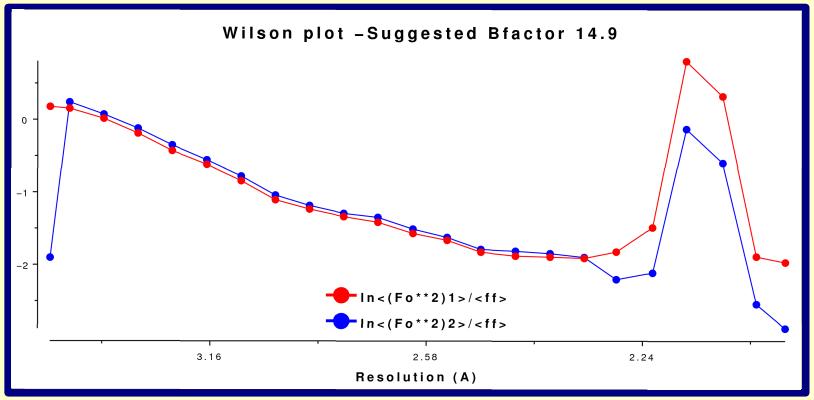
Ice-rings - 2



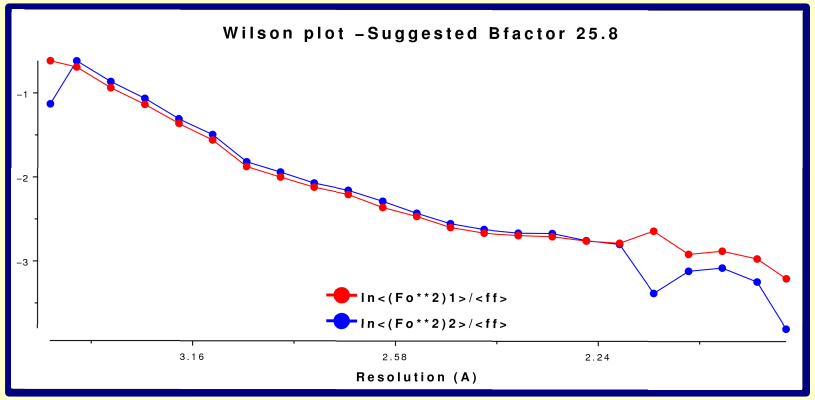
original data

Q: does it make a difference which dataset to use in refinement?

2.15 Å

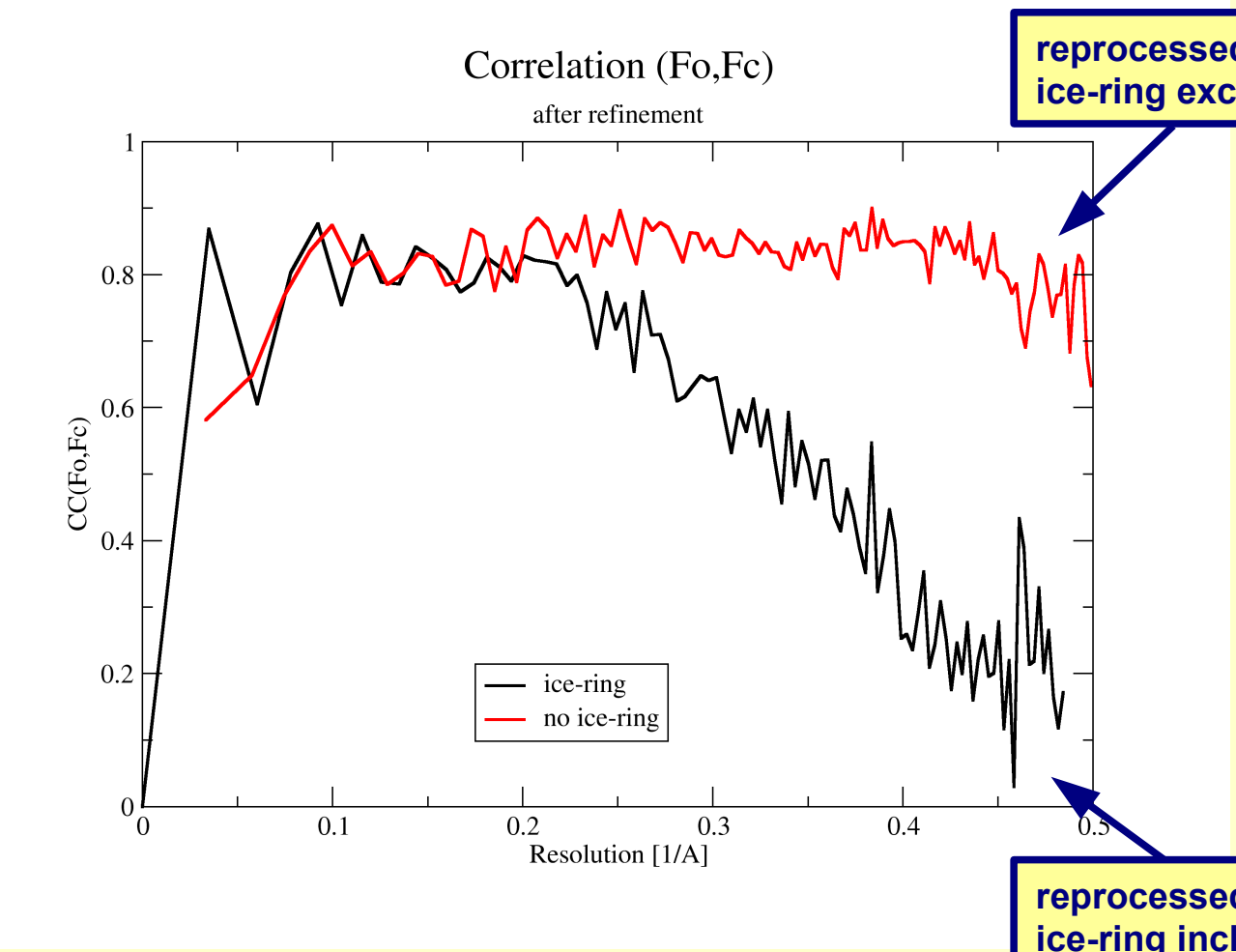


reprocessed **2.06 Å**

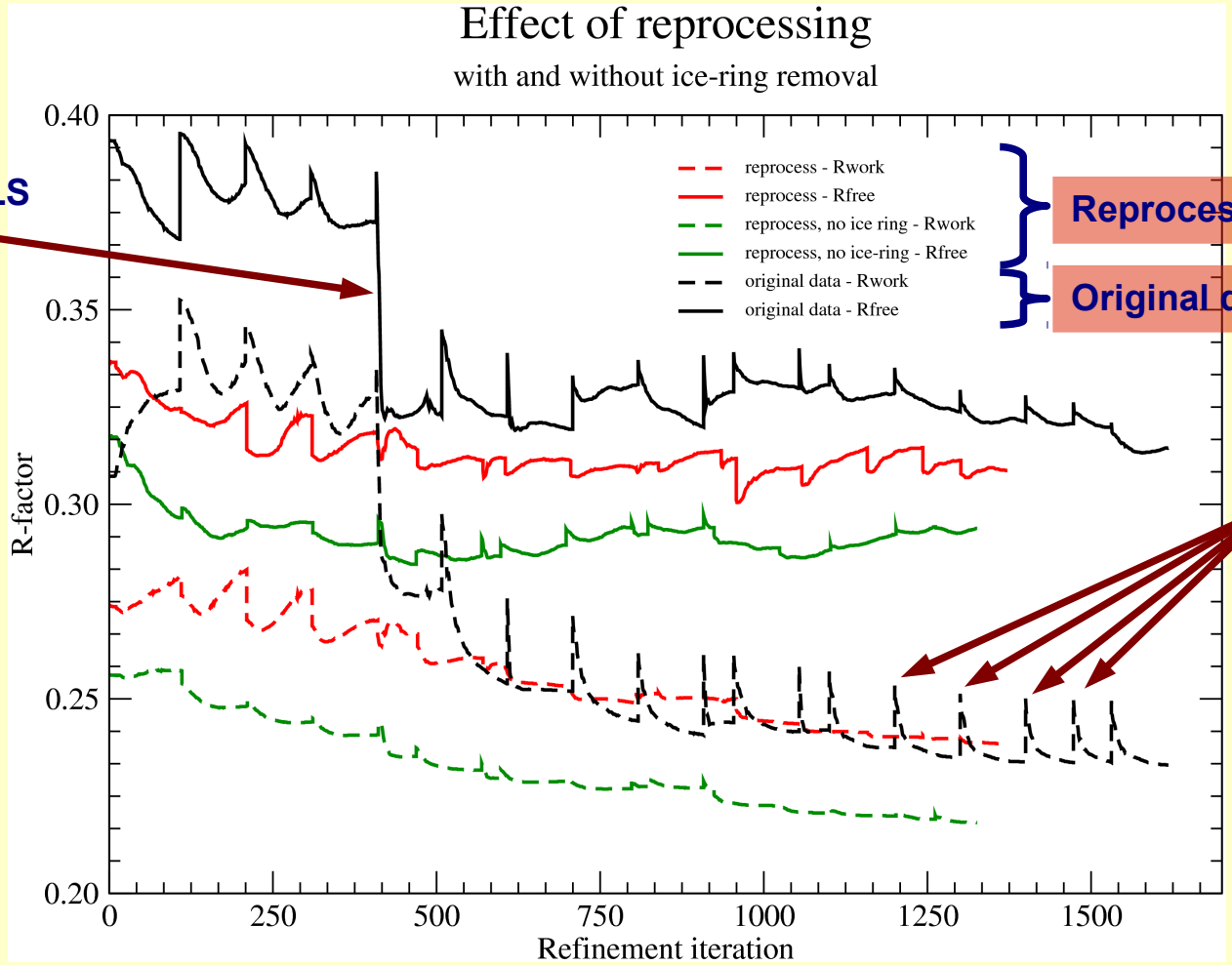


reprocessed, ice-ring excluded **2.00 Å**

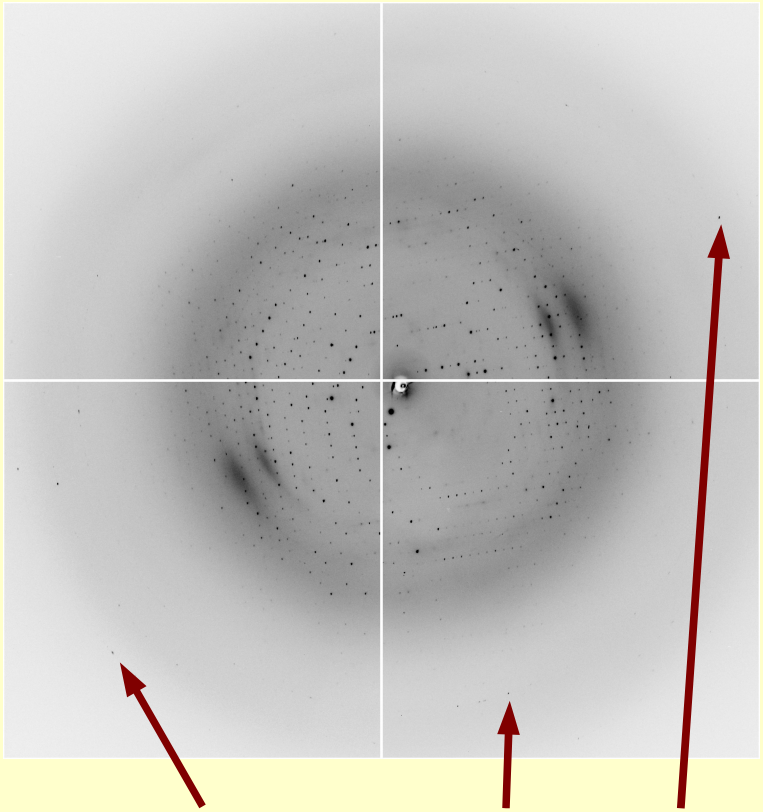
Ice-rings - 3


Correlation (Fo,Fc)
after refinement
CC(Fo,Fc)
Resolution [1/A]
ice-ring
no ice-ring
reprocessed
ice-ring excluded
reprocessed
ice-ring included

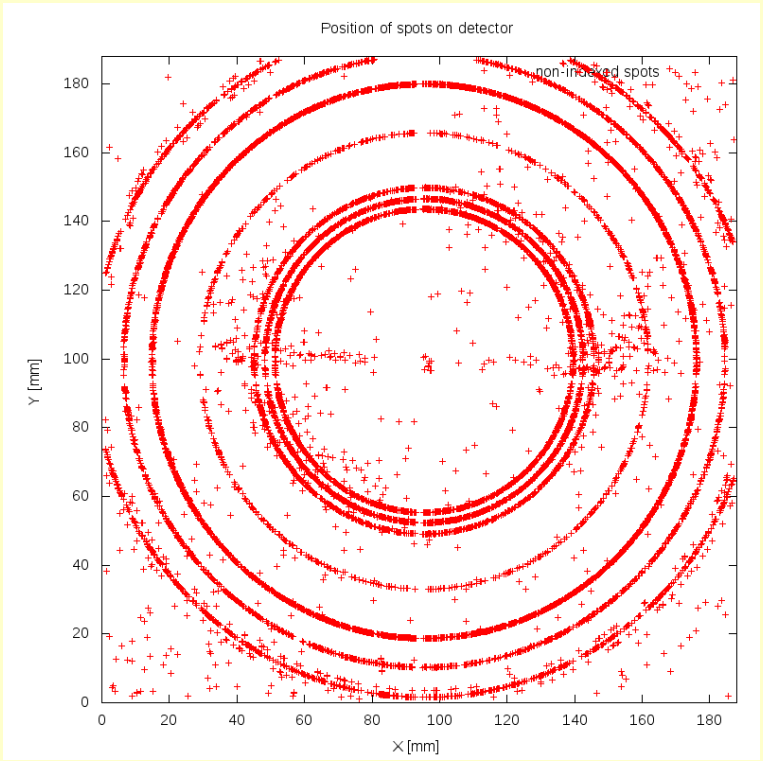
Ice-rings - 4


Effect of reprocessing
with and without ice-ring removal
0.40
0.35
0.30
0.25
0.20
R-factor
0
250
500
750
1000
1250
1500
Refinement iteration
reprocess - Rwork
reprocess - Rfree
reprocess, no ice ring - Rwork
reprocess, no ice-ring - Rfree
original data - Rwork
original data - Rfree
Reprocessed data
Original data
Switch on TLS
Redo bulk solvent mask

Ice-rings - 5



very weak ice spots visible
in region with no/weak diffraction



unindexed spots
(over all images)

Ice rings - 6

analysing unindexed spots against resolution (and compare to known values):

Resolution [A] :	no. of spots			
3.92 - 3.89 :	**1698 spots with score=**	**0.945**	**known ice-ring resolution**
3.69 - 3.66 :	**1753 spots with score=**	**0.909**	**known ice-ring resolution**
3.46 - 3.44 :	**1156 spots with score=**	**0.650**	**known ice-ring resolution**
3.37 - 3.36 :	22 spots with score=	0.867	
2.72 - 2.72 :	21 spots with score=	1.235	
2.68 - 2.67 :	**587 spots with score=**	**0.621**	**known ice-ring resolution**
2.48 - 2.47 :	28 spots with score=	2.544	
2.26 - 2.25 :	**3335 spots with score=**	**0.763**	**known ice-ring resolution**
2.20 - 2.19 :	21 spots with score=	1.150	
2.16 - 2.16 :	26 spots with score=	0.691	
2.14 - 2.13 :	23 spots with score=	0.440	
2.11 - 2.11 :	22 spots with score=	0.819	
2.08 - 2.07 :	**1615 spots with score=**	**0.698**	**known ice-ring resolution**
2.05 - 2.03 :	45 spots with score=	0.994	known ice-ring resolution
1.98 - 1.95 :	**202 spots with score=**	**0.782**	**known ice-ring resolution**
1.93 - 1.92 :	**1021 spots with score=**	**0.618**	**known ice-ring resolution**
1.90 - 1.88 :	**145 spots with score=**	**0.811**	**known ice-ring resolution**
1.83 - 1.83 :	33 spots with score=	2.107	
1.77 - 1.76 :	47 spots with score=	1.453	
1.72 - 1.72 :	22 spots with score=	0.299	known ice-ring resolution
1.70 - 1.70 :	25 spots with score=	0.366	known ice-ring resolution
1.62 - 1.61 :	26 spots with score=	1.016	

Low resolution in experimental phasing - 1

Problem: poor phasing, very low resolution structure

List of rejected reflexions:

0	**0**	**2**	**-22.54234**
0	0	8	-9.35818
0	1	1	-12.82681
0	**1**	**2**	**-68.16851**
0	1	6	-10.13897
0	1	9	-8.98388
0	**2**	**1**	**-146.59354**
0	3	15	-8.94883
0	3	20	-9.90736
...			
0	34	6	-9.33750
0	34	11	-9.64502
1	**0**	**1**	**-132.88499**
1	**0**	**2**	**-14.15716**
1	0	3	-10.23035
1	0	7	-9.55071
1	0	24	-8.93068
1	1	0	-15.43390
1	**1**	**1**	**-629.47577**
1	**1**	**2**	**-105.49634**
1	**2**	**0**	**-17.00902**
1	2	1	-10.81201
1	7	16	-9.41314
1	17	2	-9.70722
...			

BIN	Dmin	Dmax	Nacen	PP_acen
1	**105.66**	**15.84**	**248**	**4.731**
2	**15.84**	**11.26**	**563**	**4.106**
3	**11.26**	**9.21**	**748**	**3.431**
4	**9.21**	**7.99**	**909**	**3.053**
5	**7.99**	**7.15**	**1037**	**2.483**
6	**7.15**	**6.53**	**1145**	**2.184**
7	**6.53**	**6.05**	**1261**	**1.610**
8	**6.05**	**5.66**	**1374**	**1.291**
9	**5.66**	**5.33**	**1461**	**1.049**
10	5.33	5.06	1533	0.906
11	5.06	4.83	1634	0.716
12	4.83	4.62	1679	0.597
13	4.62	4.44	1787	0.502
14	4.44	4.28	1839	0.407
15	4.28	4.13	1925	0.340
16	4.13	4.00	1992	0.301
17	4.00	3.88	2057	0.275
18	3.88	3.77	2110	0.259
19	3.77	3.67	1551	0.206
20	3.67	3.58	617	0.179
OVERALL			27470	1.126

SHARP: Fortelle, E. de la & Bricogne, G. (1997). In Methods in Enzymology, Vol. 276. Macromolecular Crystallography Part A. C.W. Carter and R.M. Sweet ed. Academic Press, San Diego, pp. 472-494.

Low resolution in experimental phasing - 2

BIN	Dmin	Dmax	Nacen	PP_acen
1	105.66	15.84	260	1.857
2	15.84	11.26	568	3.470
3	11.26	9.21	756	3.027
4	9.21	7.99	915	2.847
5	7.99	7.15	1054	2.331
6	7.15	6.53	1146	2.148
7	6.53	6.05	1266	1.584
8	6.05	5.66	1380	1.287
9	5.66	5.33	1469	1.047
10	5.33	5.06	1551	0.907
11	5.06	4.83	1653	0.718
12	4.83	4.62	1713	0.599
13	4.62	4.44	1806	0.503
14	4.44	4.28	1855	0.408
15	4.28	4.13	1961	0.343
16	4.13	4.00	2009	0.303
17	4.00	3.88	2080	0.276
18	3.88	3.77	2142	0.260
19	3.77	3.67	1564	0.203
20	3.67	3.58	624	0.173
OVERALL			27772	1.095

?

all reflections

BIN	Dmin	Dmax	Nacen	PP_acen
1	105.66	15.84	248	4.731
2	15.84	11.26	563	4.106
3	11.26	9.21	748	3.431
4	9.21	7.99	909	3.053
5	7.99	7.15	1037	2.483
6	7.15	6.53	1145	2.184
7	6.53	6.05	1261	1.610
8	6.05	5.66	1374	1.291
9	5.66	5.33	1461	1.049
10	5.33	5.06	1533	0.906
11	5.06	4.83	1634	0.716
12	4.83	4.62	1679	0.597
13	4.62	4.44	1787	0.502
14	4.44	4.28	1839	0.407
15	4.28	4.13	1925	0.340
16	4.13	4.00	1992	0.301
17	4.00	3.88	2057	0.275
18	3.88	3.77	2110	0.259
19	3.77	3.67	1551	0.206
20	3.67	3.58	617	0.179
OVERALL			27470	1.126

excluding rejections

Low resolution in experimental phasing - 3

BIN	Dmin	Dmax	Nacen	PP_acen
1	**105.66**	**15.84**	**260**	**1.857**
2	**15.84**	**11.26**	**568**	**3.470**
3	**11.26**	**9.21**	**756**	**3.027**
4	**9.21**	**7.99**	**915**	**2.847**
5	**7.99**	**7.15**	**1054**	**2.331**
6	**7.15**	**6.53**	**1146**	**2.148**
7	**6.53**	**6.05**	**1266**	**1.584**
8	**6.05**	**5.66**	**1380**	**1.287**
9	**5.66**	**5.33**	**1469**	**1.047**
10	5.33	5.06	1551	0.907
11	5.06	4.83	1653	0.718
12	4.83	4.62	1713	0.599
13	4.62	4.44	1806	0.503
14	4.44	4.28	1855	0.408
15	4.28	4.13	1961	0.343
16	4.13	4.00	2009	0.303
17	4.00	3.88	2080	0.276
18	3.88	3.77	2142	0.260
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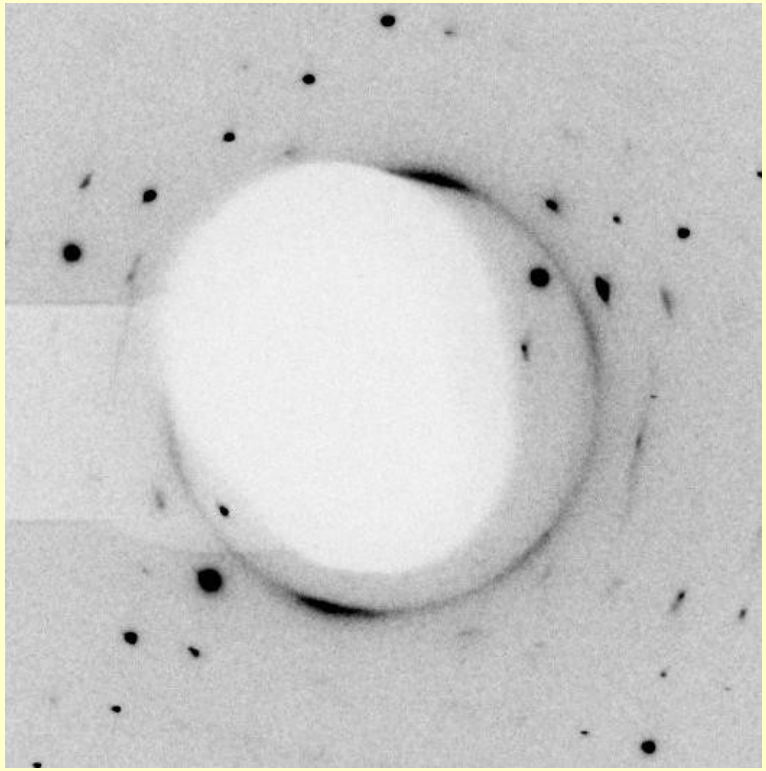
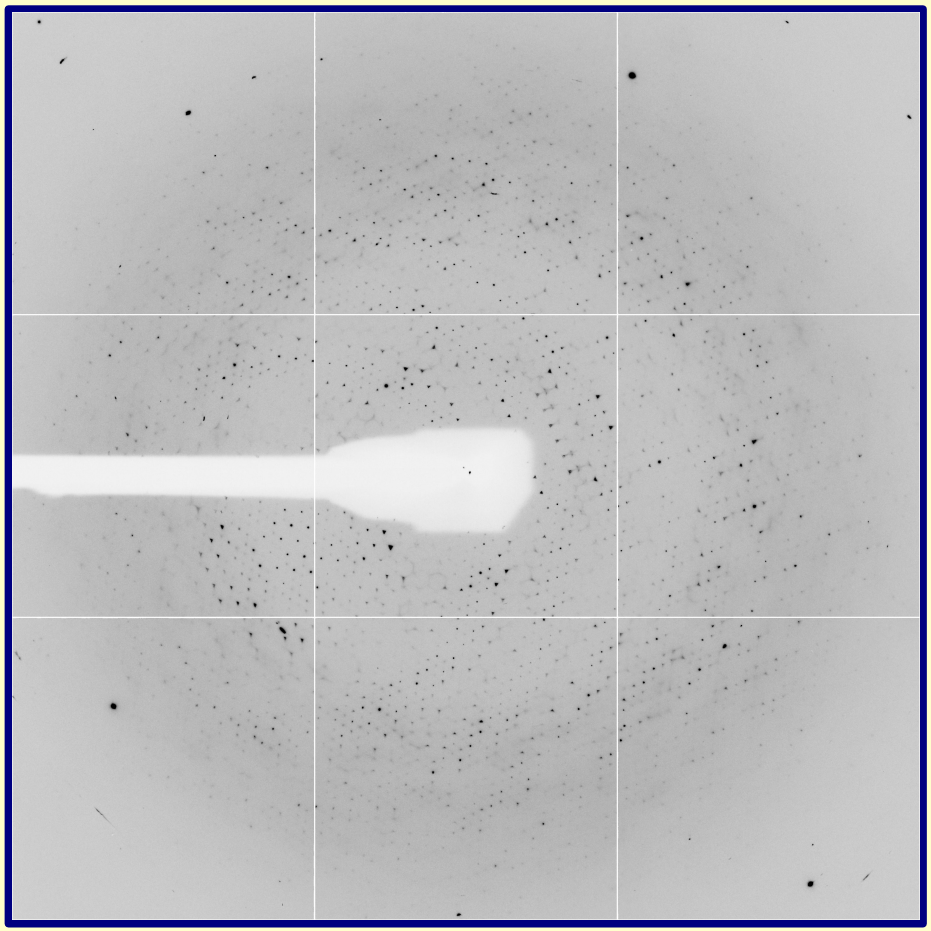
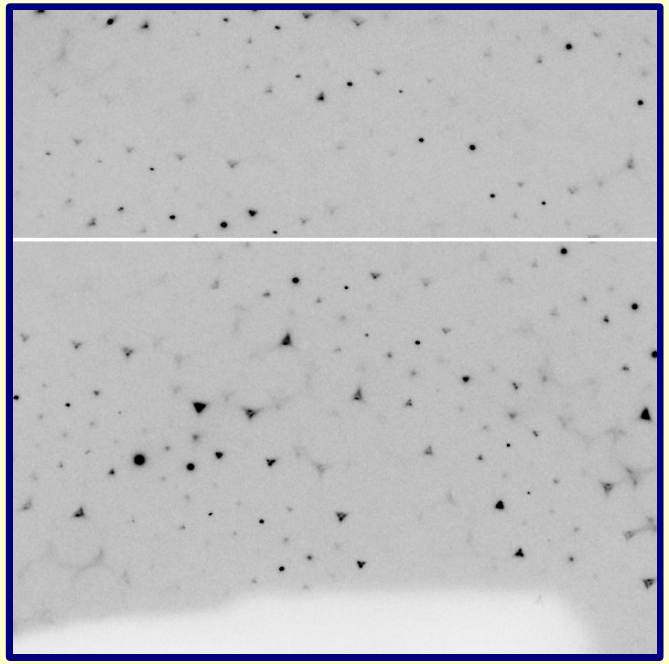
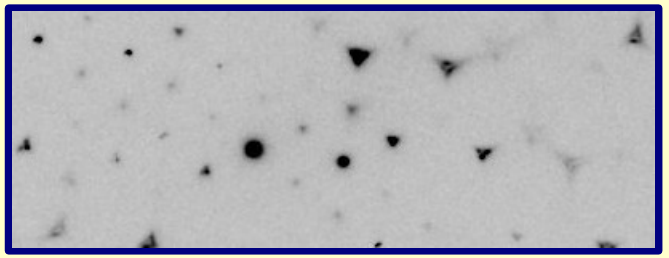
OVERALL			27772	1.095



Low resolution in experimental phasing - 4



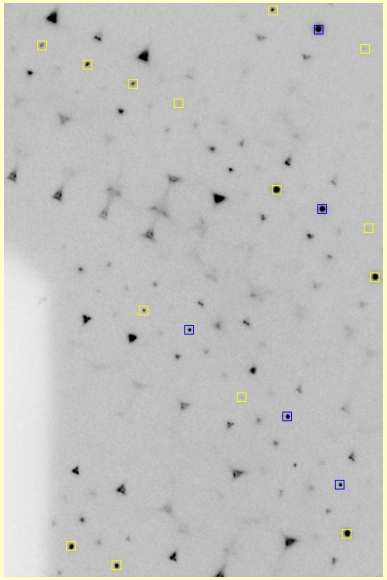




MOSFLM: A. Leslie (1992). Joint CCP4-ESF-EAMCB Newsletter on Protein Crystallography 26.

Low resolution in experimental phasing - 5

	Overall	InnerShell	OuterShell
Low resolution limit	22.74	22.74	2.74
High resolution limit	2.61	8.22	2.61
Rmerge	0.076	0.040	0.442
Ranom	0.050	0.047	0.226
Rmeas (within I+/I-)	**0.084**	**0.045**	**0.501**
Rmeas (all I+ & I-)	**0.095**	**0.062**	**0.507**
Total number of observations	55451	1563	5622
Total number unique	5465	182	745
Mean(I)/sd(I)	22.5	82.0	4.6
Completeness	99.7	93.9	99.1
Multiplicity	10.1	8.6	7.5
Anomalous completeness	98.8	92.3	93.0
Anomalous multiplicity	5.3	5.0	4.0
DelAnom correlation between half-sets	**0.609**	**0.792**	**0.024**
Mid-Slope of Anom Normal Probability	1.467		
ditto (all data)	2.172		



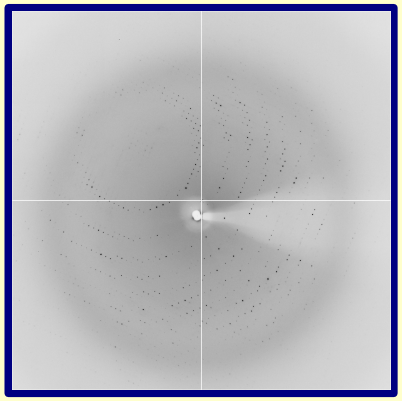
Looks great: strong anomalous signal ... but there is a small problem:

fraction of unit cell occupied by atoms = 1.276 <=====

Outliers (ROGUES) - 1

Summary data for Project: Test Crystal: A Dataset: 0.9772A

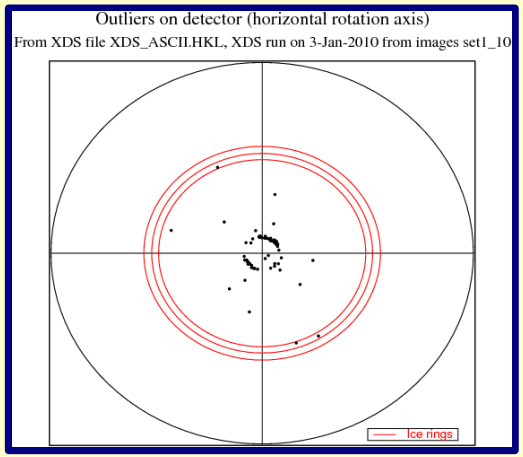
	Overall	InnerShell	OuterShell
Low resolution limit	79.86	79.86	2.16
High resolution limit	2.05	6.49	2.05
Rmerge	0.123	0.078	0.444
Ranom	0.032	0.017	0.314
Rmeas (within I+/I-)	0.130	0.082	0.604
Rmeas (all I+ & I-)	0.129	0.082	0.562
Rpim (within I+/I-)	0.130	0.025	0.406
Rpim (all I+ & I-)	0.129	0.019	0.306
Total number of observations	288942	13992	5686
Total number unique	19939	755	2051
Mean(I)/sd(I)	17.0	39.5	2.0
Completeness	92.3	100.0	67.0
Multiplicity	14.5	18.5	2.8



Inverse beam experiment: 5 images a 1°

360° of data, H32

Problem: unable to solve



Scala: P.R.Evans (2005). Scaling and assessment of data quality. Acta Cryst. D62, 72-82.

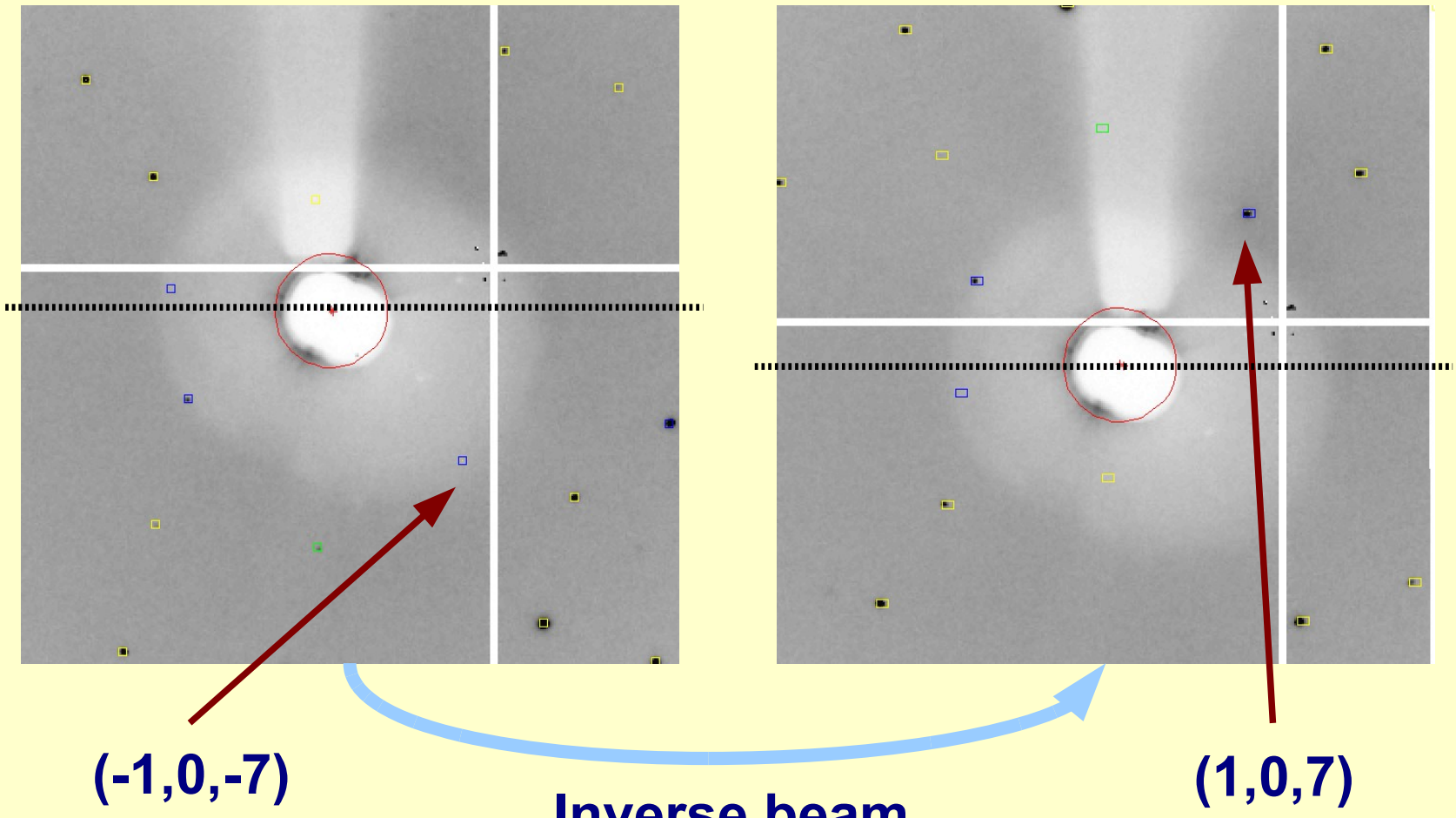
Outliers (ROGUES) - 2

```
The ROGUES file contains all rejected reflections (flag "*", "@" for I+- rejects, "#" for Emax rejects)
    TotFrc = total fraction, fulls (f) or partials (p)
    Flag I+ or I- for Bijvoet classes
    DelI/sd = (Ihl - Mn(I)others)/sqrt[sd(Ihl)**2 + sd(Mn(I))**2]
   h   k   l     h   k   l  Batch      I  sigI    E  TotFrc Flag Scale   LP   DelI/sd d(A)   Xdet   Ydet    Phi
   (measured)     (unique)

   1   0  -2     1   0  -2   1142     -6     2  0.00  1.00f  I+  1.043  0.017    0.6 59.05  998.9 1144.0  321.5
  -1   1  -2     1   0  -2   1171     -6     2  0.00  0.96f  I+  1.066  0.006    0.8 59.05  968.2 1121.4  350.4
  -1   1  -2     1   0  -2   2168     17     2  0.11  1.00f *I+  1.041  0.006    9.0 59.05  968.9 1093.7  167.6
   0  -1  -2     1   0  -2   1076     -6     2  0.00  1.00f  I+  1.045  0.015    0.6 59.05  985.3 1140.6  255.9
   0  -1  -2     1   0  -2   2075     17     2  0.11  1.00f *I+  1.037  0.015   11.0 59.05  986.0 1075.7   74.8
   0   1   2     1   0  -2   1075    -10     2  0.00  1.00f  I-  1.036  0.015   -2.2 59.05 1019.9 1076.1  254.8
                   Weighted mean     -7

   1   0   7     1   0   7   1108    361    34  0.51  1.00f *I+  1.055  0.030   10.3 21.15 1080.9 1042.5  287.6
  -1   0  -7     1   0   7   1112    362    34  0.51  1.00f *I-  1.051  0.030   10.3 21.15  924.1 1173.4  291.7
  -1   0  -7     1   0   7   2108      2     5  0.04  1.00f  I-  1.028  0.030   -9.4 21.15  925.6 1040.8  107.4
  -1   1   7     1   0   7   1113    316    30  0.47  1.00f *I+  1.045  0.042   10.1 21.15 1050.3 1017.7  292.6
   1  -1  -7     1   0   7   1116    339    32  0.49  1.00f *I-  1.052  0.042   10.2 21.15  954.6 1198.1  295.6
   1  -1  -7     1   0   7   2113     -5     6  0.00  1.00f *I-  1.046  0.041   -1.6 21.15  956.7 1016.6  112.5
   0  -1   7     1   0   7   1136    443    47  0.56  0.91f  I+  1.051  0.036    9.4 21.15 1067.0 1028.6  315.7
   0   1  -7     1   0   7   1140    436    46  0.56  1.00f *I-  1.050  0.036    9.3 21.15  937.7 1186.7  319.2
                   Weighted mean      7
...
```

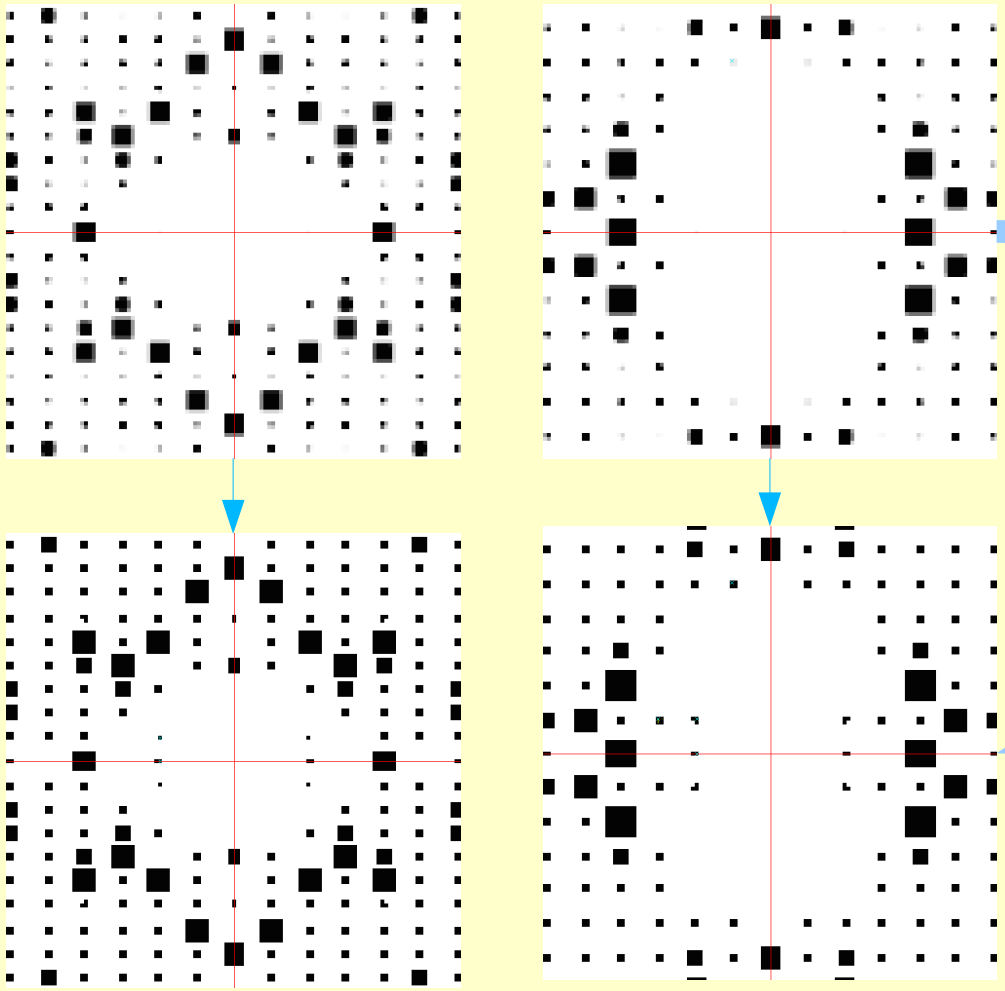
Inverse beam: **'phi-0'** **= batches 1001-1180**

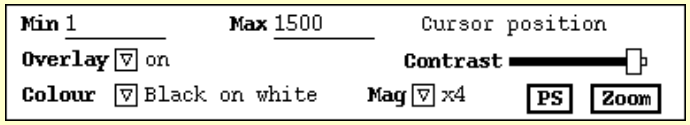
'phi-180' **= batches 2001-2180**

Outliers (ROGUES) - 3

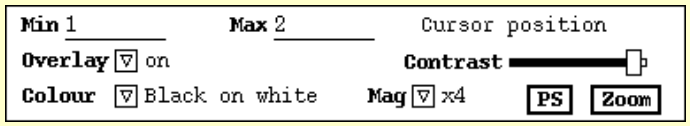


Outliers (ROGUES) - 4





Change **Max** value
in *hklview* interface



Outliers (ROGUES) - 5

WARNING : there are serious differences between 2 amplitudes from different datasets (as judged by analysing E values). If these appear only in specific resolution ranges or shells you might be able to improve results by restricting e.g. low resolution. Here is a list of the reflections that look **suspicious**:

H	K	L	Reso	w1	w2	w3 (all)	
-2	0	4	10.75	126.22	137.03	**2.31**	*
-3	1	3	12.15	**3.12**	-	**581.69**	*

NOTE : 4 reflexions have large anomalous differences:

H	K	L	FMID	SMID	DANO	SANO	ABS(DANO)/FMID	
-3	1	12	203.27	5.43	398.98	7.68	1.96	*
-2	2	12	79.28	2.86	-150.88	4.05	1.90	*
-2	6	17	177.12	8.44	-259.31	11.94	1.46	
-1	1	2	28.28	2.17	-43.53	3.07	1.54	

WARNING : We will remove 2 reflexions with a ABS(DANO)/FMID ratio > 1.9

Analysis/correction becomes more difficult once data is merged

Indexing - 1

Why does **indexing fails**? Some of the possible reasons:

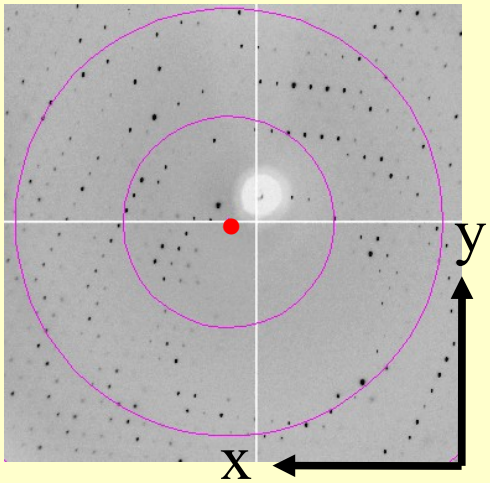
- Wrong information
  - **beam centre**
  - rotation axis
  - oscillation range
  - wavelength, distance
- Not enough spots
- **Too many spots**
- Inspect images:
  - Beam centre
  - Loons
  - Overlaps
  - Ice-rings

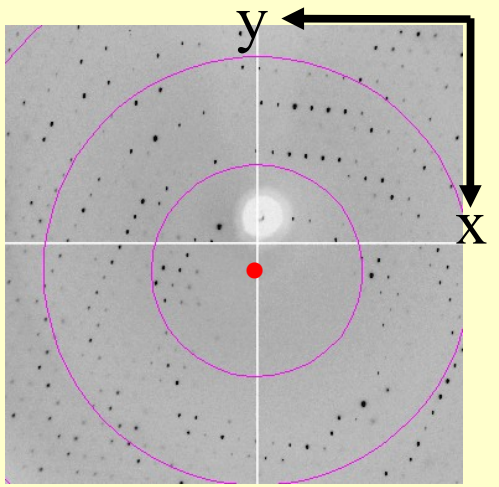
two main reasons (?)

- ice-rings
- multiple lattices
- radiation damage (cell change)
- crystal slippage

Indexing - 2

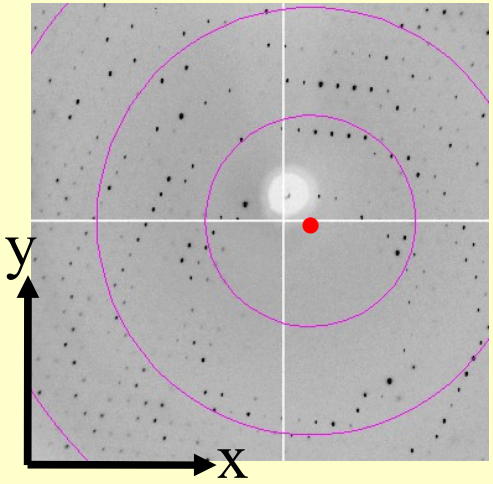
(X,Y)
header

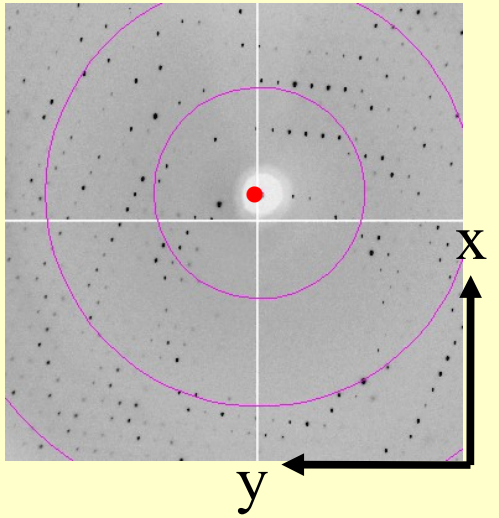




(Y,-X)

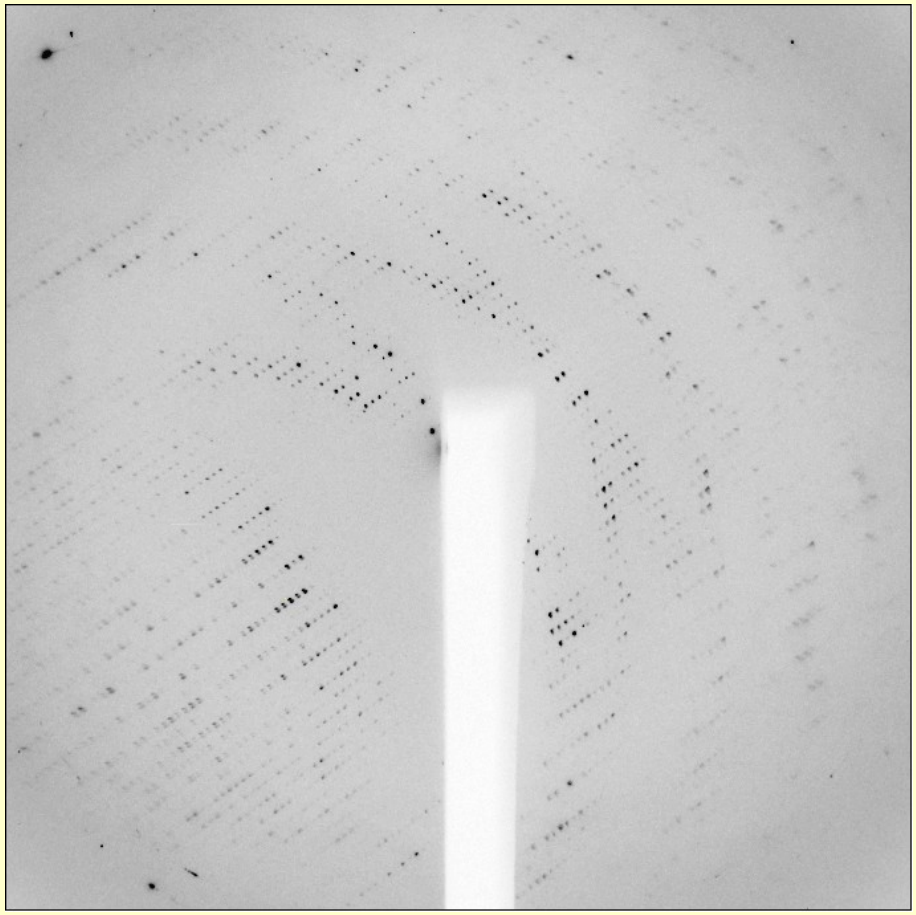
(-X,Y)

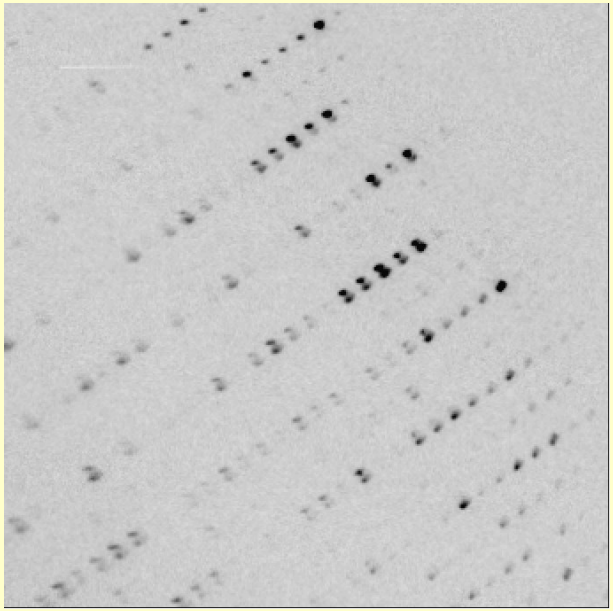




(Y,X)
correct

Multiple lattices - 1





Herbst-Irmer, R. & Sheldrick, G. M. (1998). Refinement of Twinned Structures with SHELXL97. Acta Cryst. B54, 443-449.

Parsons, S. (2003). Introduction to twinning. Acta Cryst. D59, 1995-2003.

Multiple lattices - 2

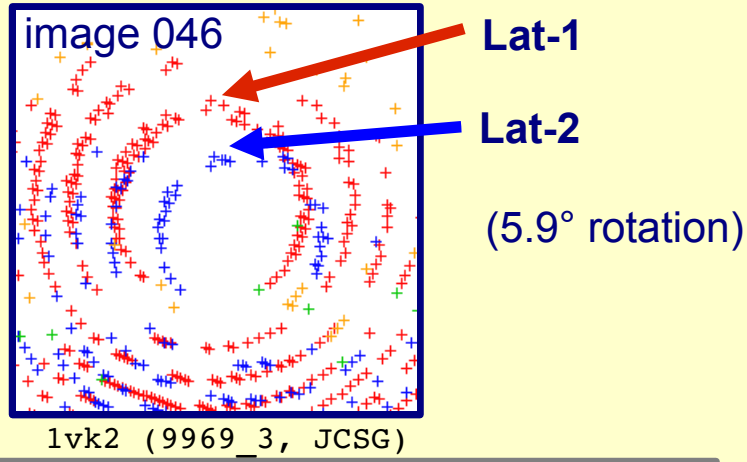
spot search and indexing using XDS

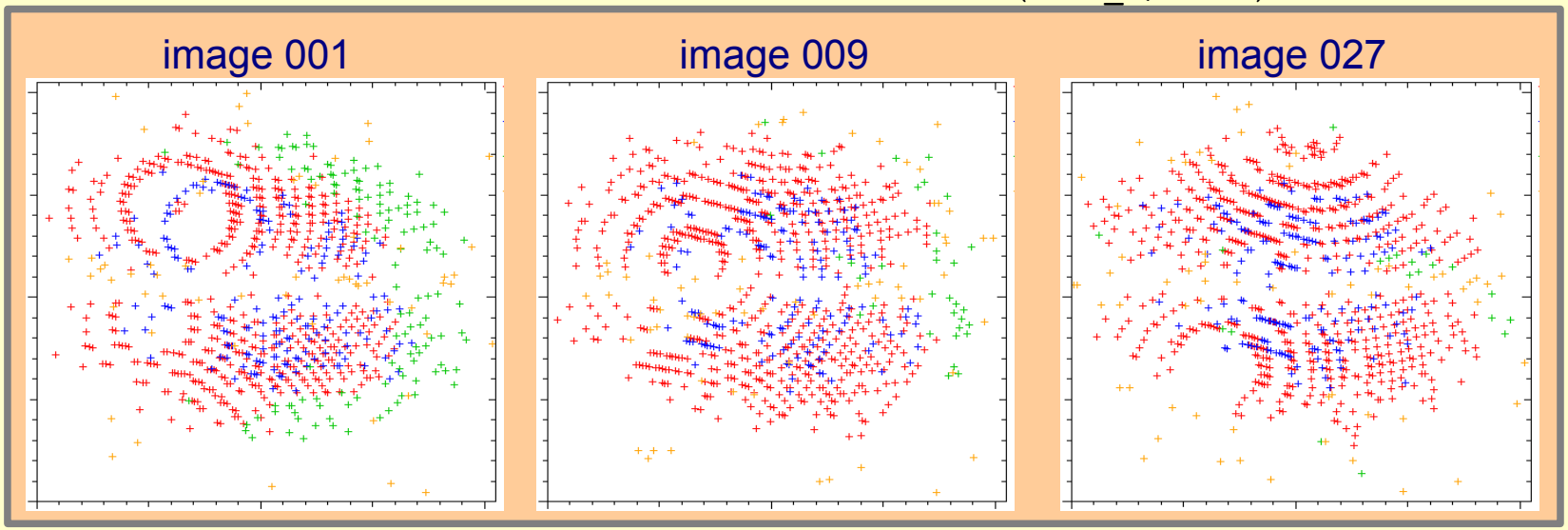
assign spots to different lattices

get best indexing for each lattice

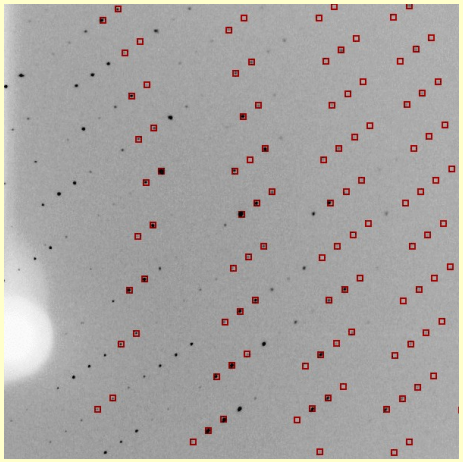
visualize different lattices for most populated images

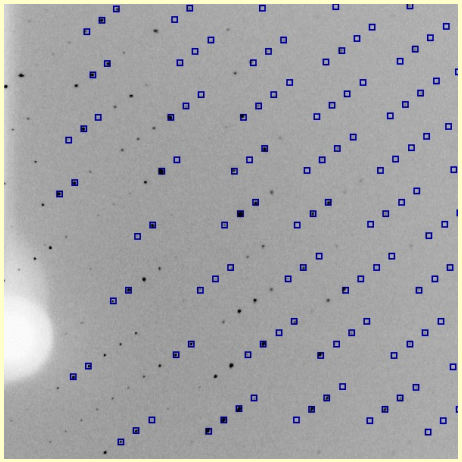
comparison of orientation matrices

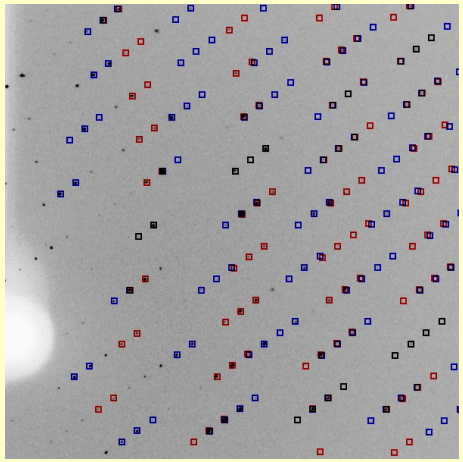




Multiple lattices - 3

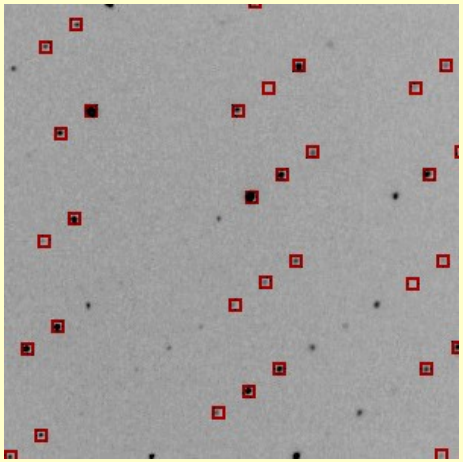


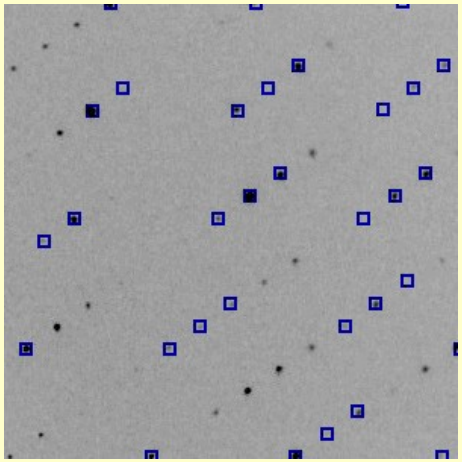


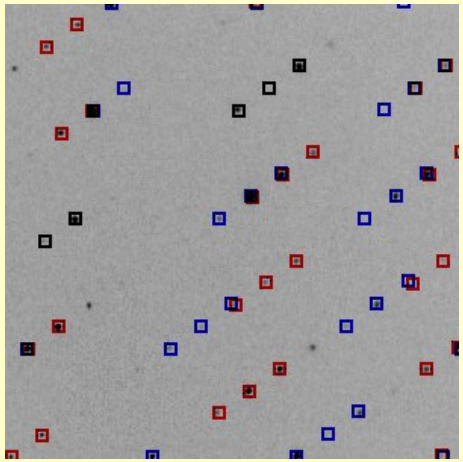


Lattice 1 → 180° → Lattice 2

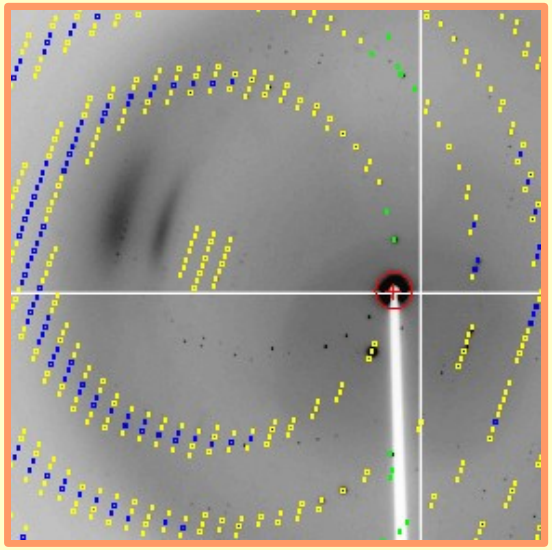
Lattice 1+2

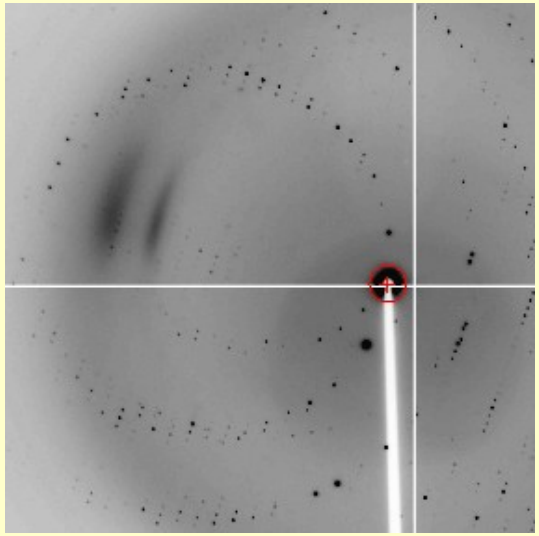


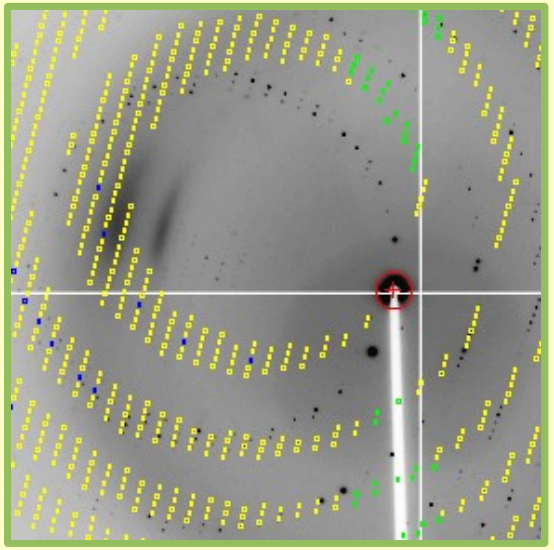




Multiple lattices - 4



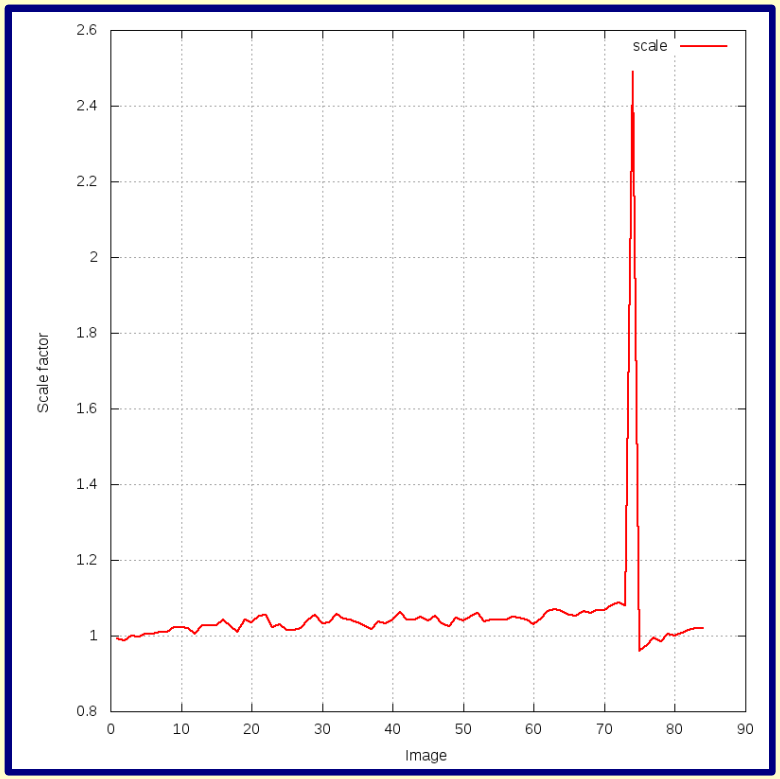


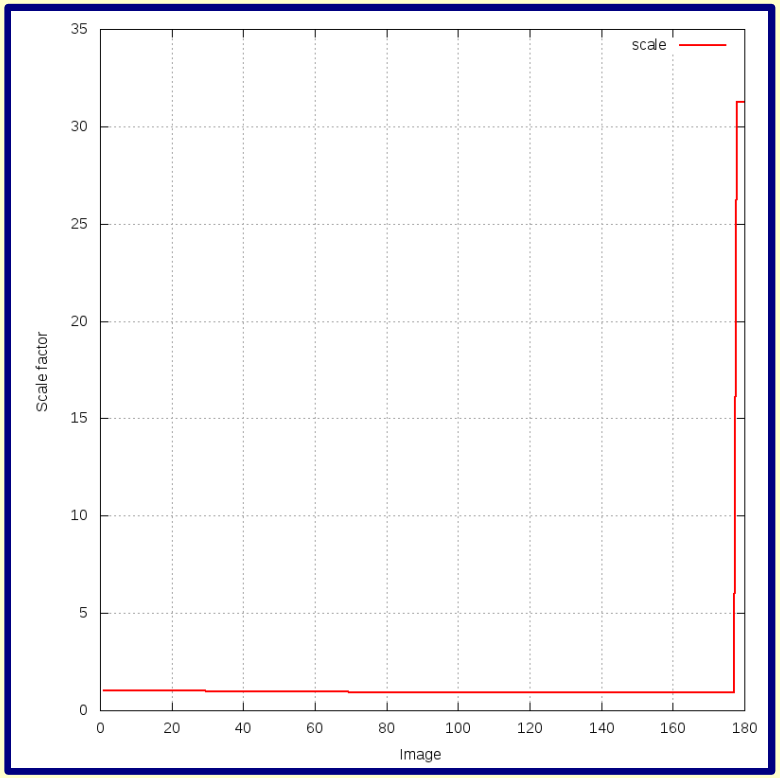


	Overall	InnerShell	OuterShell
Low res [A]	43.14	43.14	2.00
High res [A]	1.90	6.01	1.90
Rmerge	0.074	0.036	0.525
Rmeas	0.087	0.048	0.656
Mean(I)/sd(I)	16.8	77.2	2.8
Completeness	98.0	97.9	87.0
Multiplicity	6.5	5.4	4.1

Overall	InnerShell	OuterShell
127.00	127.00	3.04
2.88	9.12	2.88
0.211	0.092	0.433
0.320	0.162	0.698
5.9	10.5	2.0
99.0	96.4	96.5
4.7	3.9	3.2

Integration - 1

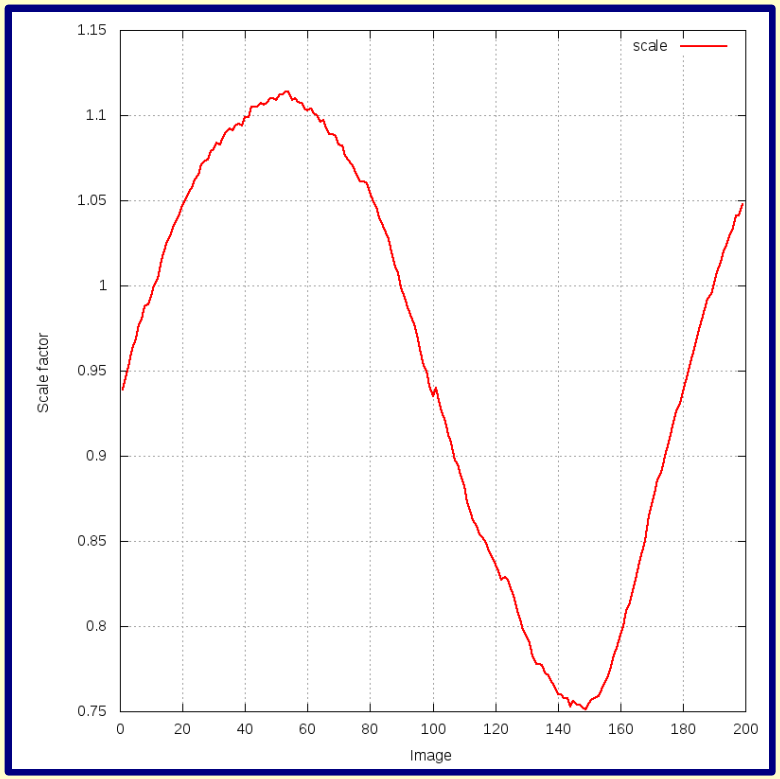




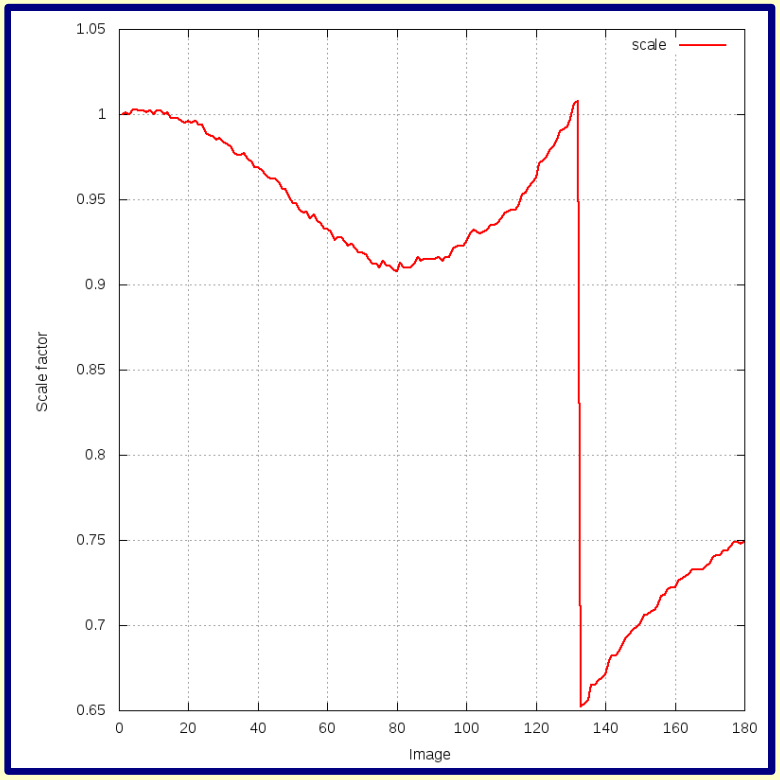
per-image scale (XDS): detect problematic images

Kabsch, W. (2001) Chapter 25.2.9. XDS in International Tables for Crystallography, Volume F.

Integration - 2



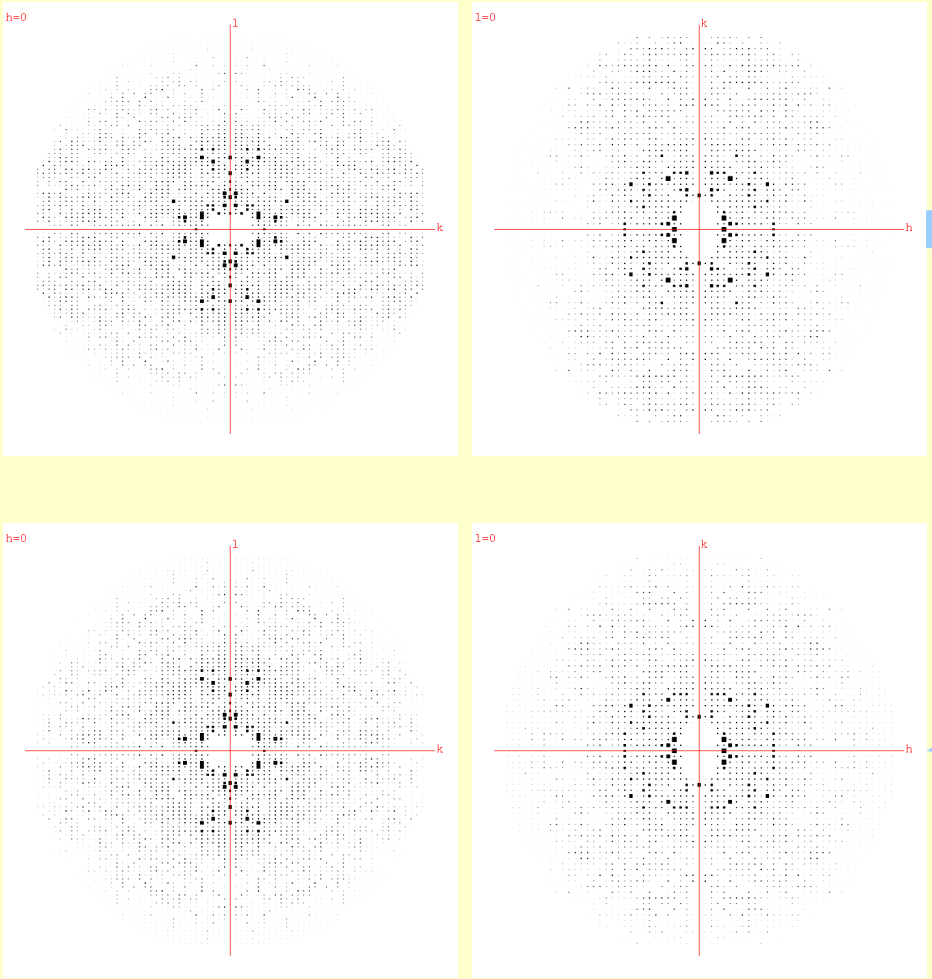
360°: plate-like crystal?
anisotropic diffraction?
poorly centred?



180°: beam dump?
fresh part of crystal?

what would be nice : movie of crystal as it rotates during data collection
for now : analyse timestamp in image header (MAR, ADSC, Pilatus, RIgaku, ...)

Anisotropy - 1



SHARP/autoSHARP

Vonrhein, C., Blanc, E., Roversi, P. & Bricogne, G. (2007). Methods Mol Biol 364, 215-30

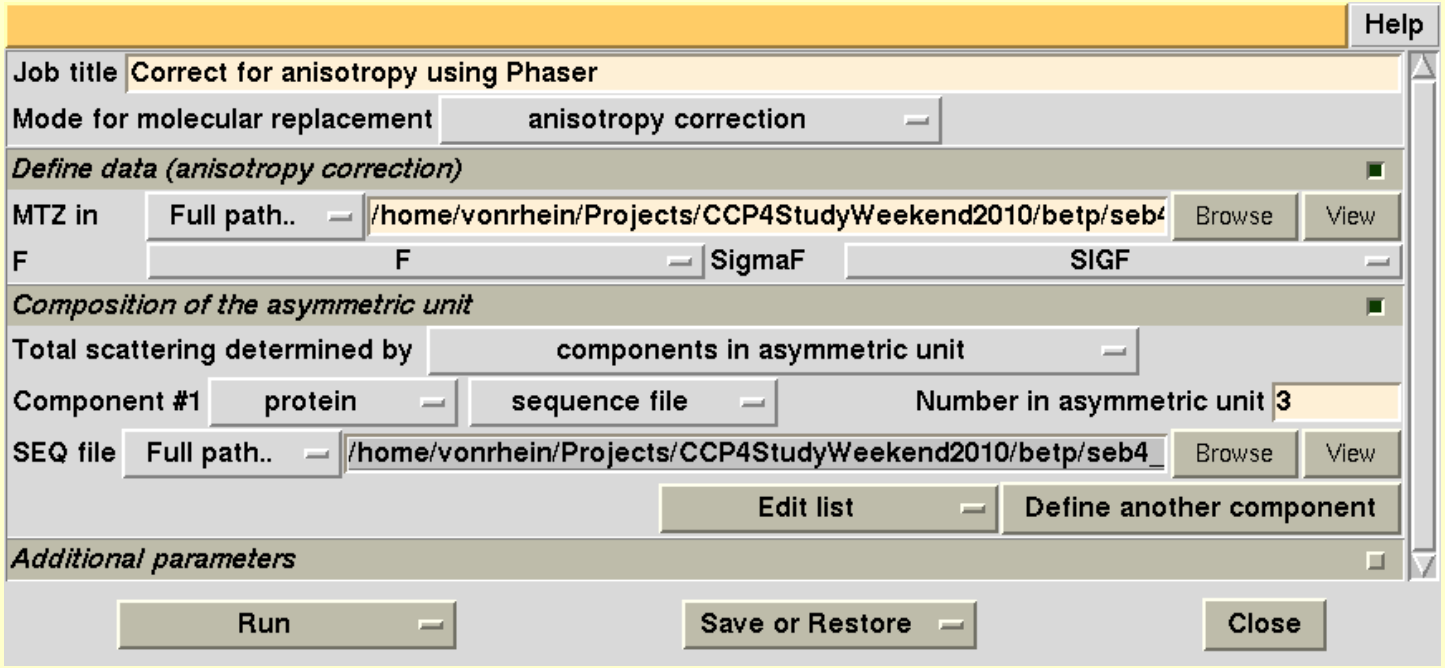
SFCHECK

A.A.Vaguine, J.Richelle, S.J.Wodak. Acta Cryst. (1999). D55, 191-205

PHASER

A. J. McCoy, R. W. Grosse-Kunstleve, P. D. Adams, M. D. Winn, L.C. Storoni and R.J. Read (2007). J. Appl. Cryst. (2007). 40, 658-674.

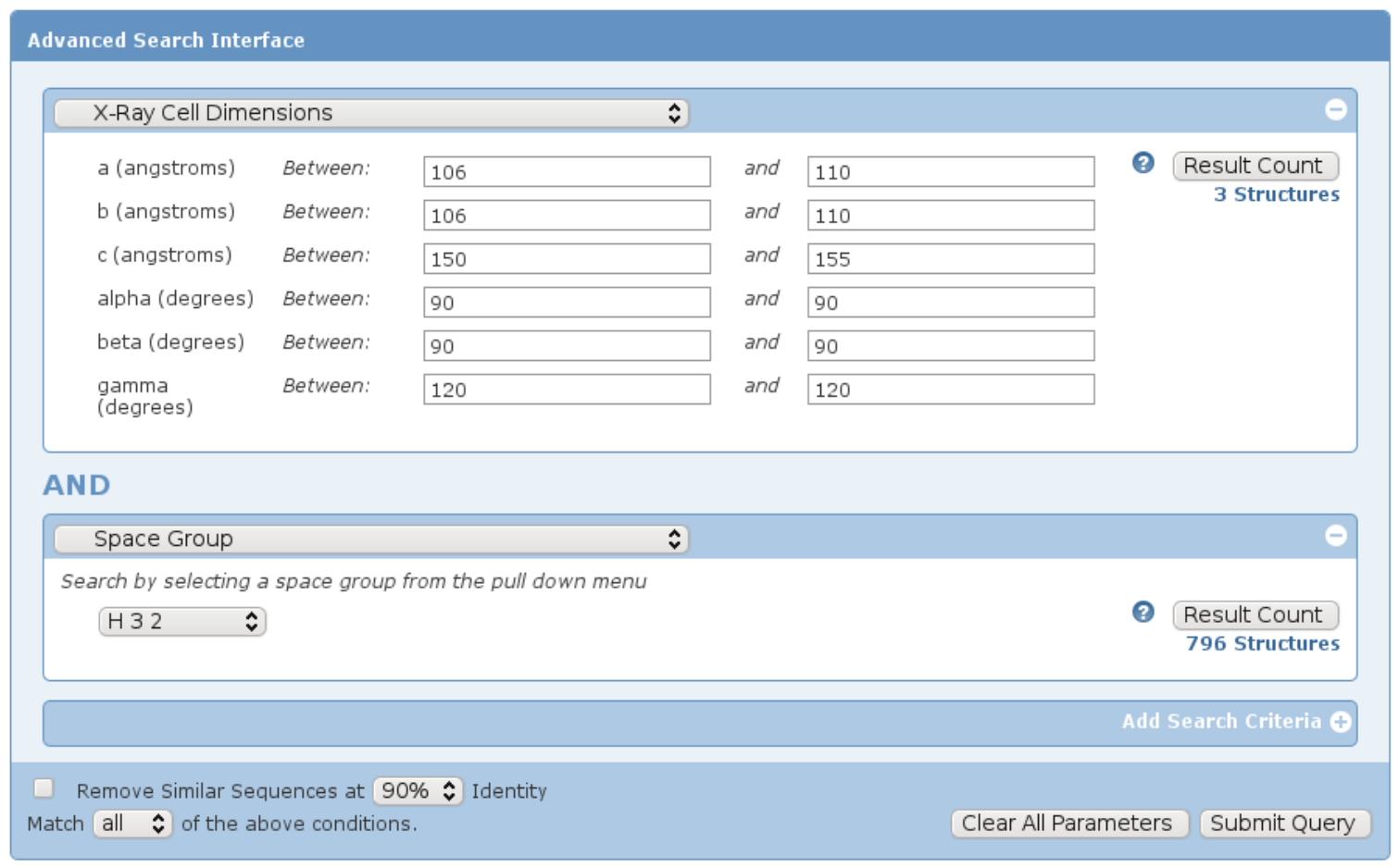
Anisotropy - 2




```
Principal components of anisotropic part of B affecting observed amplitudes:
 eigenB (A^2)  direction cosines (orthogonal coordinates)
    41.578           1.0000   0.0000   0.0000
    23.639          -0.0000   0.0000   1.0000
   -65.218          -0.0000   1.0000  -0.0000
```

can be crucial in density modification and/or automatic building

Expect the unexpected - 1



Expect the unexpected - 2

INORGANIC PYROPHOSPHATASE FROM ESCHERICHIA COLI WITH THREE MAGNESIUM IONS

DOI: 10.2210/pdb1ipw/pdb

1IPW Display Files ▾ | Download Files ▾ | Print this Page | Share this Page

Primary Citation

Crystallographic identification of metal-binding sites in Escherichia coli inorganic pyrophosphatase.
Kankare, J., Salminen, T., Lahti, R., Cooperman, B.S., Baykov, A.A., Goldman, A.
(1996) Biochemistry **35:** 4670-4677

PubMed: 8664256 DOI: 10.1021/bi952637e
Search Related Articles in PubMed

PubMed Abstract:

We report refined crystal structures of the hexameric soluble inorganic pyrophosphatase from Escherichia coli (E-PPase) to R-factors of 18.3% and 17.1% at 2.2 and 2.3 angstroms, respectively. Both structures contain two independent monomers in the asymmetric unit of an R32 ... [Read More & Search PubMed Abstracts]

Molecular Description Hide

Classification: Hydrolase
Structure Weight: 39267.92

Molecule: SOLUBLE INORGANIC PYROPHOSPHATASE
Polymer: 1 Type: polypeptide(L) Length: 175
Chains: A, B
EC#: 3.6.1.1

Source Hide

Polymer: 1
Scientific Name: Escherichia coli

Ligand Chemical Component Hide

Identifier	Name	Formula	Interaction View	Links
MG	MAGNESIUM ION	Mg	Ligand Explorer	

Derived Data Hide

- SCOP Classification v1.75 - (2 Domains)
- CATH Classification v3.2.0 - (2 Domains)
- PFAM Classification - (2 Domains)
- GO Terms - (9 Terms)

Reset Layout

Biological Assembly

More Images...

View in Jmol | SimpleViewer | Other Viewers | Protein Workshop

Biological assembly assigned by authors

Deposition Summary Hide

Authors: Kankare, J.A., Goldman, A.

Deposition:	1996-03-04
Release:	1997-08-20
Last Modified (REVDAT):	2009-02-24

Experimental Details Hide

Method: X-RAY DIFFRACTION
Experimental Data: N/A

Resolution[Å]:	2.30
R-Value:	0.171 (obs.)
R-Free:	0.239
Space Group:	H 3 2

Unit Cell:

Length [Å]	Angles [°]
a = 109.40	α = 90.00
b = 109.40	β = 90.00
c = 154.30	γ = 120.00

Acknowledgements

Global Phasing, Cambridge (UK):

Gérard Bricogne, C. Flensburg, P. Keller, W. Paciorek, A. Sharff, O. Smart,
T. Womack: SHARP/autoSHARP, BUSTER, autoPROC

Program developers:

MOSFLM: Andrew Leslie & Harry Powell (MRC/LMB Cambridge)

SCALA/POINTLESS: Phil Evans (MRC/LMB Cambridge)

XDS: Wolfgang Kabsch (MPI Heidelberg) & Kay Diederichs (Universität Konstanz)

Users and test data:

Global Phasing Consortium members

Felix Rey, Marija Backovic, Joseph Cockburn, Stephane Duquerroy, Sebastien Igonet, Thomas Krey, Carlos Massayuki, Alejandra Tortorici, Marie-Christine Vaney, James Voss (Institut Pasteur, Paris)

Susanne Ressl, Christine Ziegler (MPI Biophysik, Frankfurt), Martin Grininger, Kornelius Zeth (MPI Biochemistry, Martinsried), Qilu Ye (Queens University, Kingston, Ontario), Andrew Mattevi (Pavia) … and many many more

The Joint Center for Structural Genomics (JCSG)