
Data processing with autoPROC and STARANISO, and requirements for the full visualisation of results via ISPyB

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Global Phasing Ltd.

MXCube/ISPyB Meeting
DLS
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autoPROC - behind the scenes

Vonrhein, C., Flensburg, C., Keller, P., Sharff, A., Smart, O., Paciorek, W., Womack, T. & Bricogne, G. (2011). Data processing and analysis with the **autoPROC** toolbox. *Acta Cryst. D67*, 293-302.

❑ Uses external programs

- **XDS/XSCALE**: Kabsch, W. *XDS. Acta Cryst. D66*, 125-132 (2010).
- **POINTLESS, AIMLESS**: Evans, P. (2006). Scaling and assessment of data quality. *Acta Cryst. D62*, 72-82.
- **CCP4**: Collaborative Computational Project, Number 4. 1994. "The CCP4 Suite: Programs for Protein Crystallography". *Acta Cryst. D50*, 760-763.

Some background information

- ❑ Deployed as 3rd party processing pipeline at multiple synchrotrons
- ❑ Data processing pipeline(s) within industry
- ❑ Needs to support
 - Fully-automated synchrotron operation
 - Different detectors (Pilatus, Eiger, CCD, Proteum, IP, ...)
 - Inhouse data processing
 - Single and multi-sweep datasets
 - Multi-wvl (interleaved wavelengths, MAD)
 - Inverse-beam (SAD)
 - Multiple positions, helical scan
 - Unsupervised processing, manual processing (expert, novice), educational tool
 - Distributed and supported software (free to academics) with ~400 active licences
- ❑ Apart from external (crystallographic) software requirements: needs to be as independent and stand-alone as possible

Reporting and interaction with users

❑ Technology

- ASCII => stdout
- HTML + PNG => summary.html
- XML => ISPyB (and internal/corporate databases)

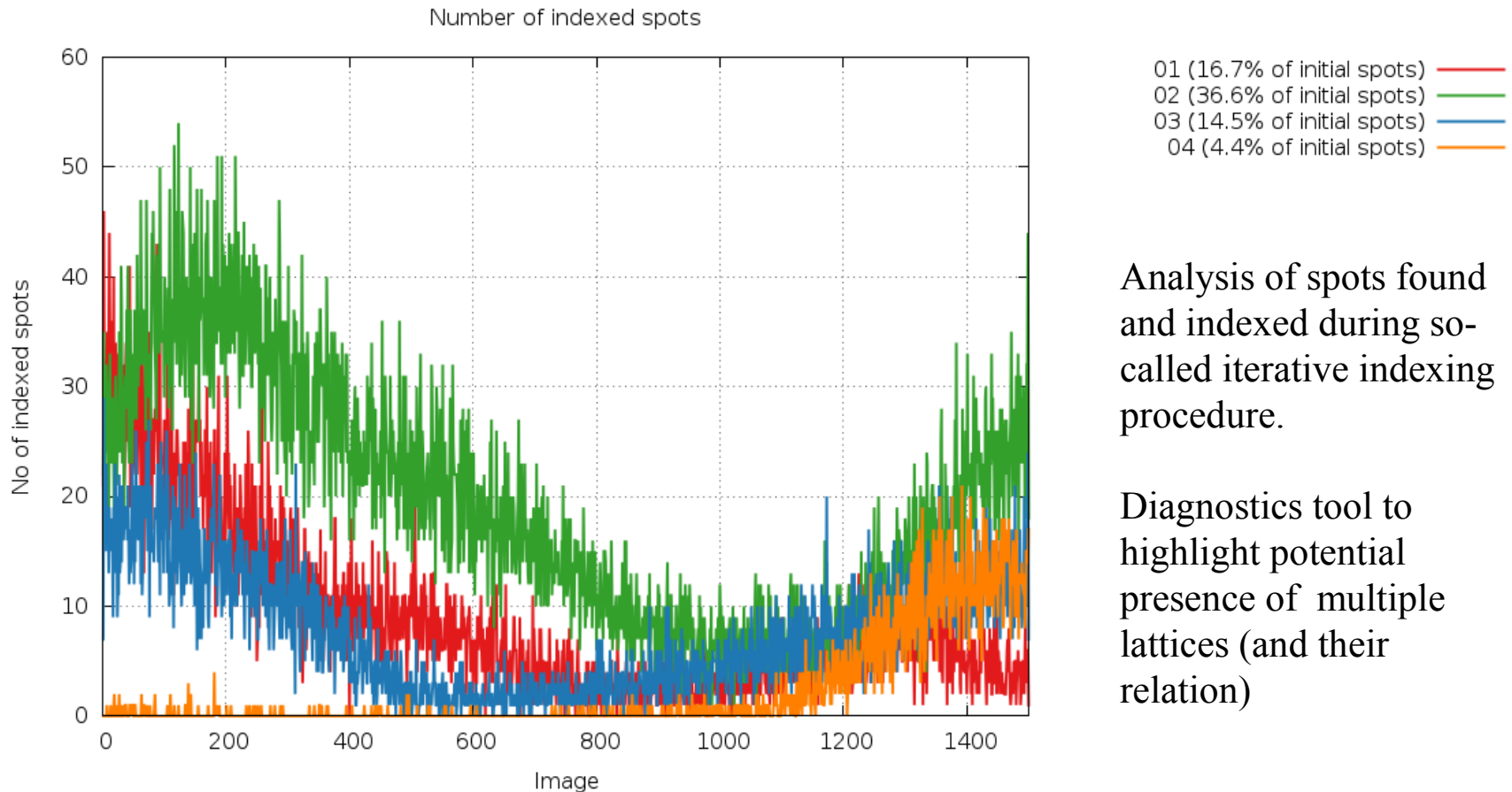
❑ Presentation

- Tables/values for archiving, harvesting, deposition
- Plots/graphs for more complex analysis, decision making, problem detection, design of (next) experiment
- XML for DB integration

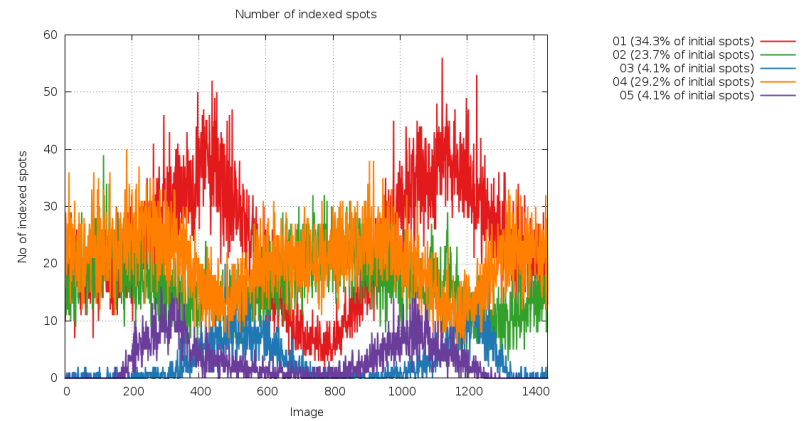
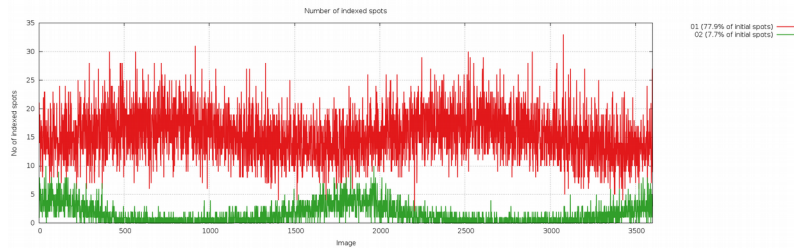
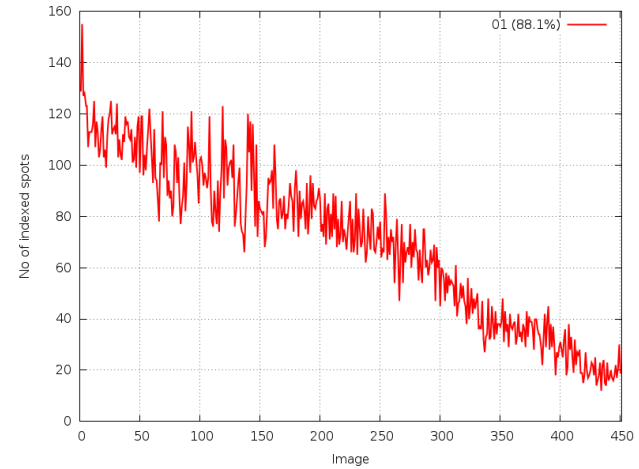
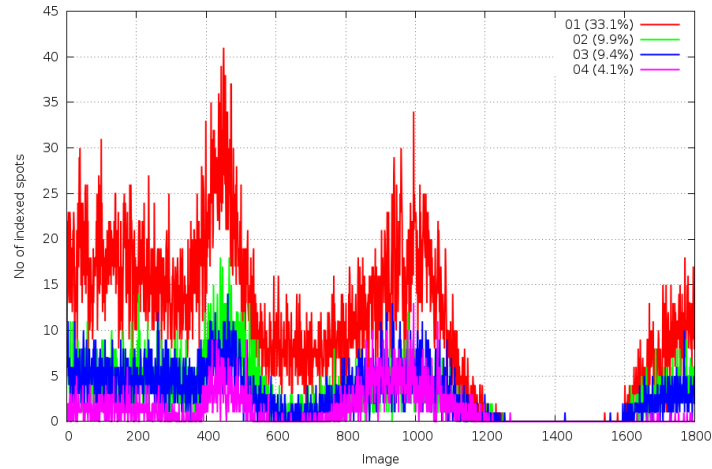
❑ The way autoPROC results are presented is based on our own understanding of the science and what we would like to present and emphasise to the user

- Ideally, this should be mirrored when autoPROC results are presented to users at synchrotron beamlines

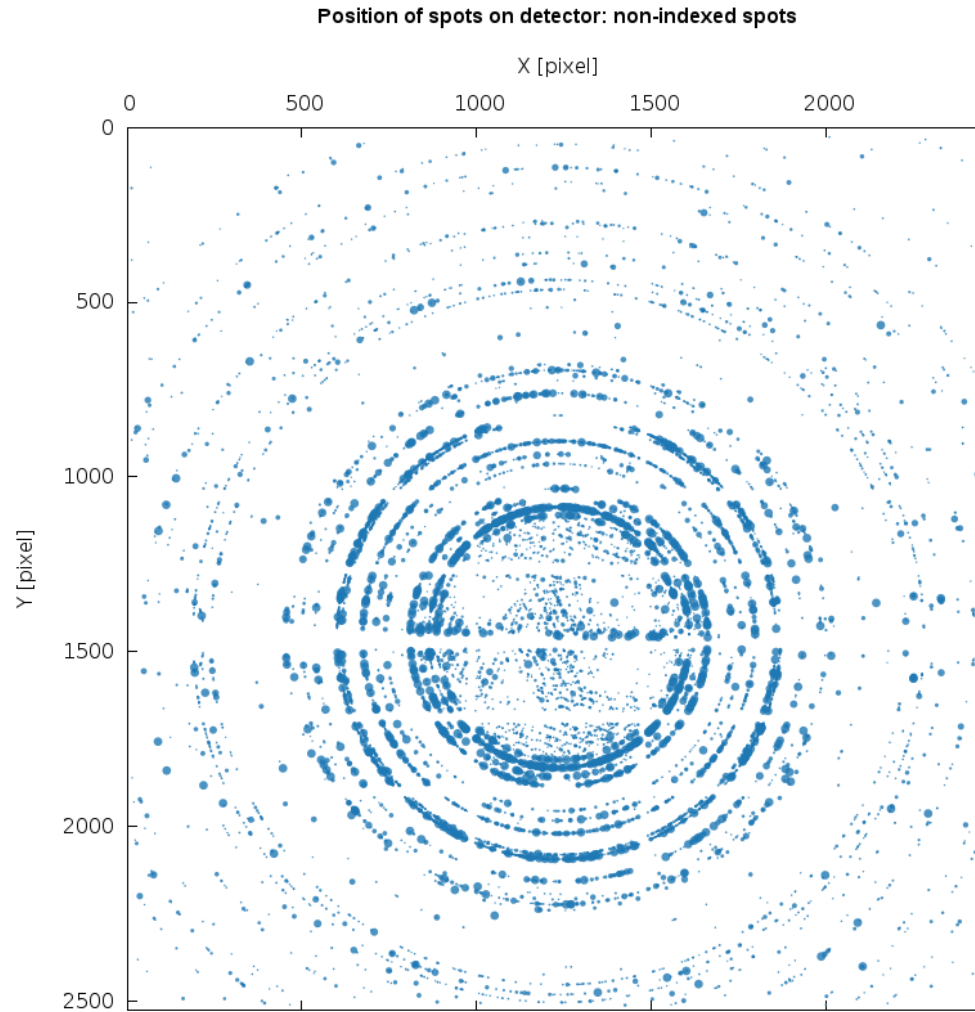
Advanced analysis of datasets



A picture is worth a thousand words

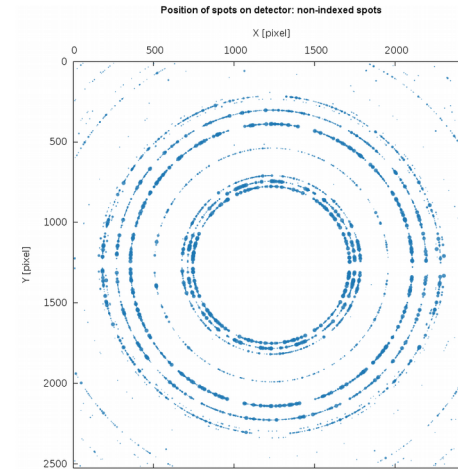
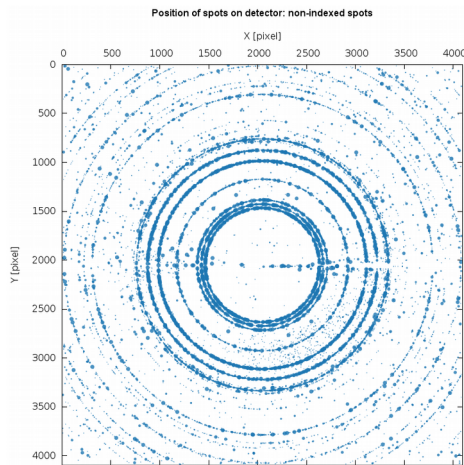
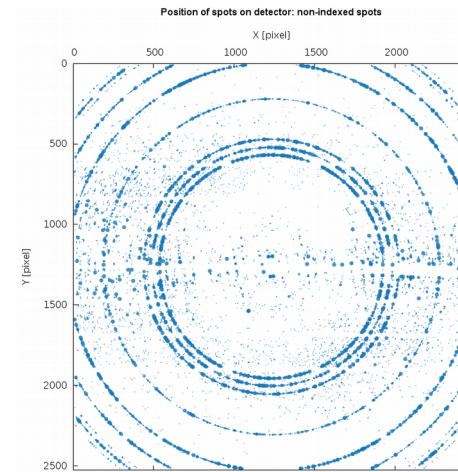
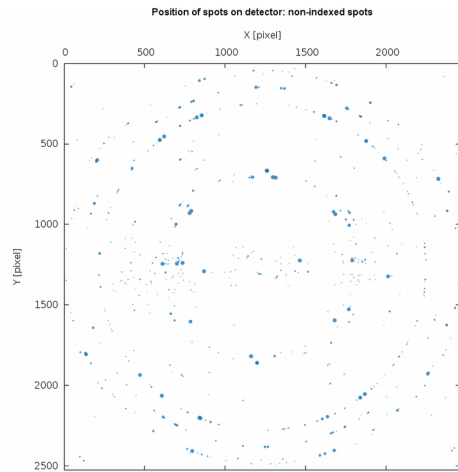


Advanced analysis of datasets

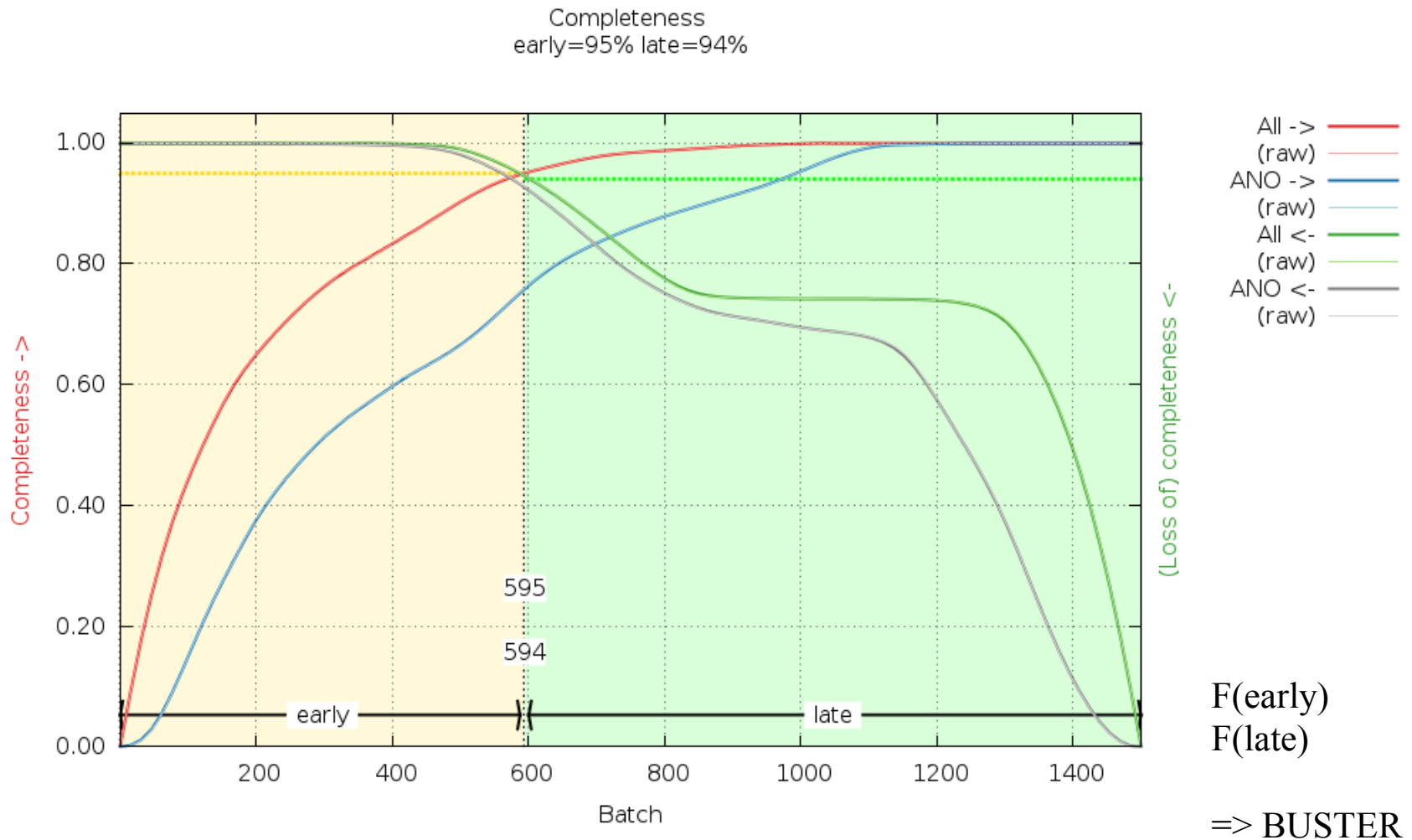


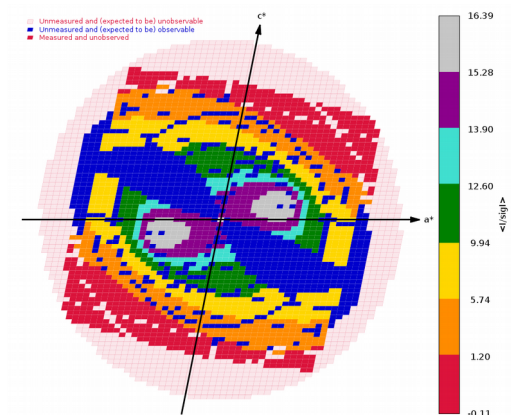
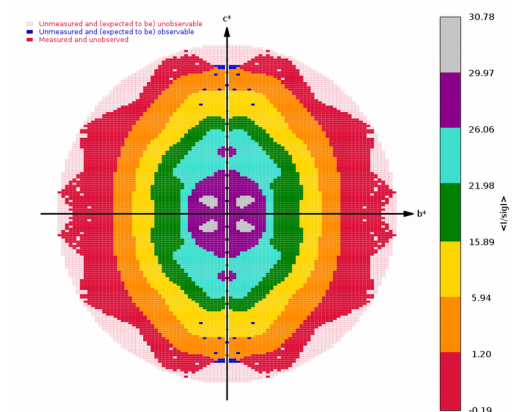
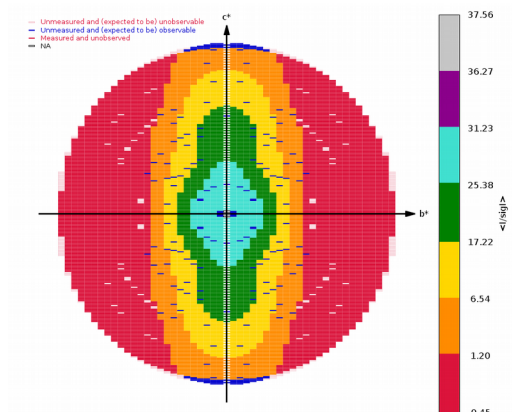
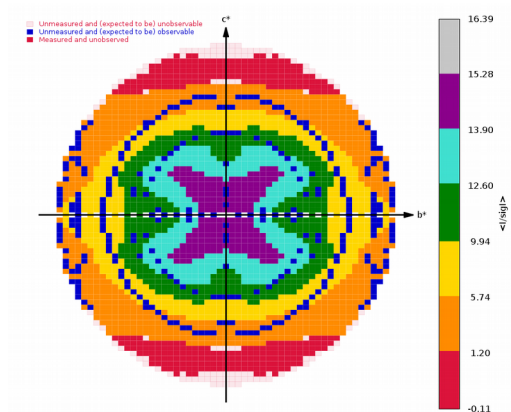
Detection of ice-rings
(which will be
automatically excluded
from processing if
obvious enough)

A picture is worth a thousand words

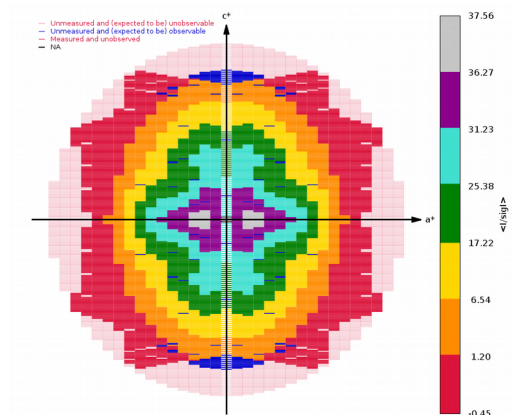


Some analysis difficult to put into numbers

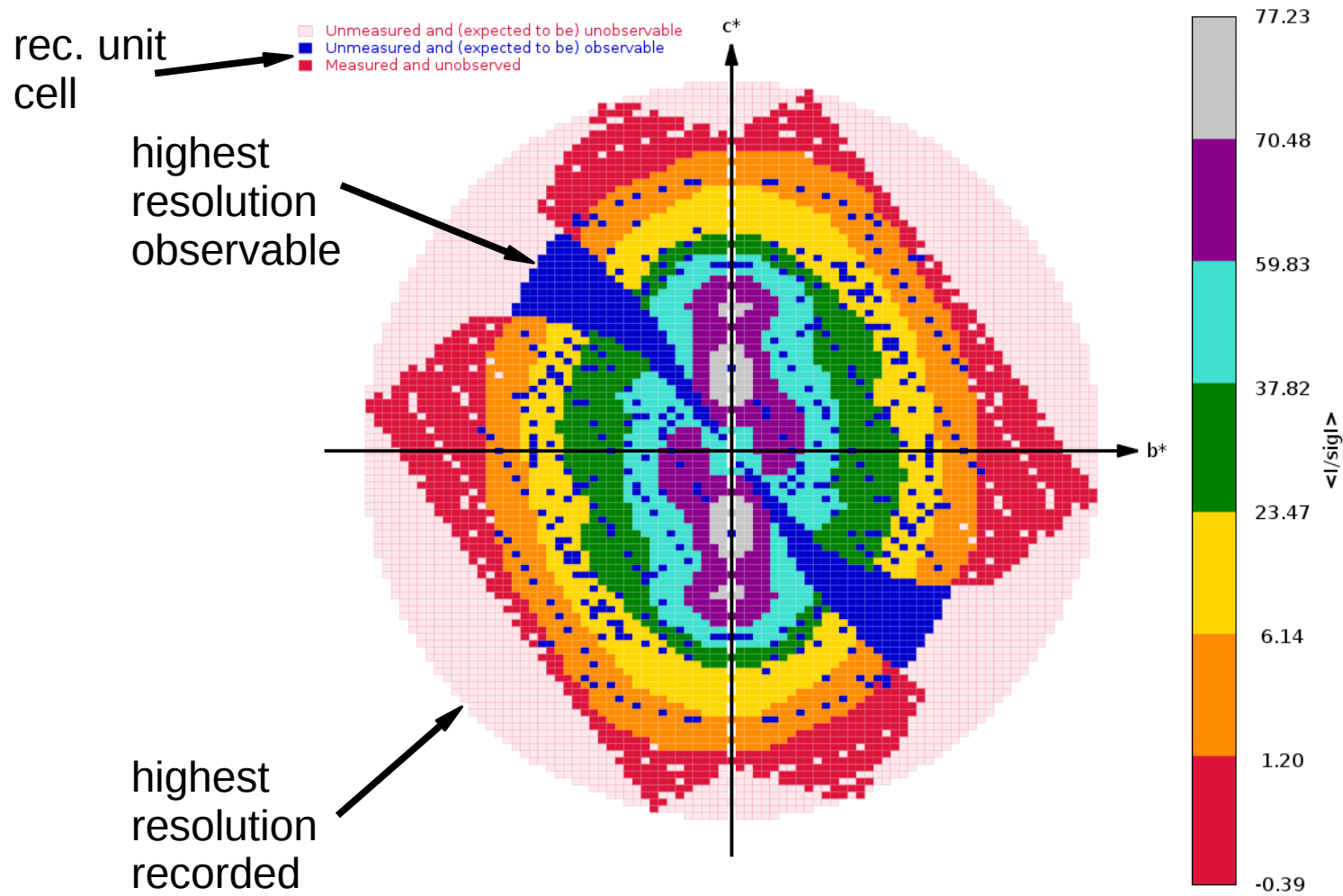




Plots of local $\langle I/\sigma_I \rangle$
for each r.l.p.



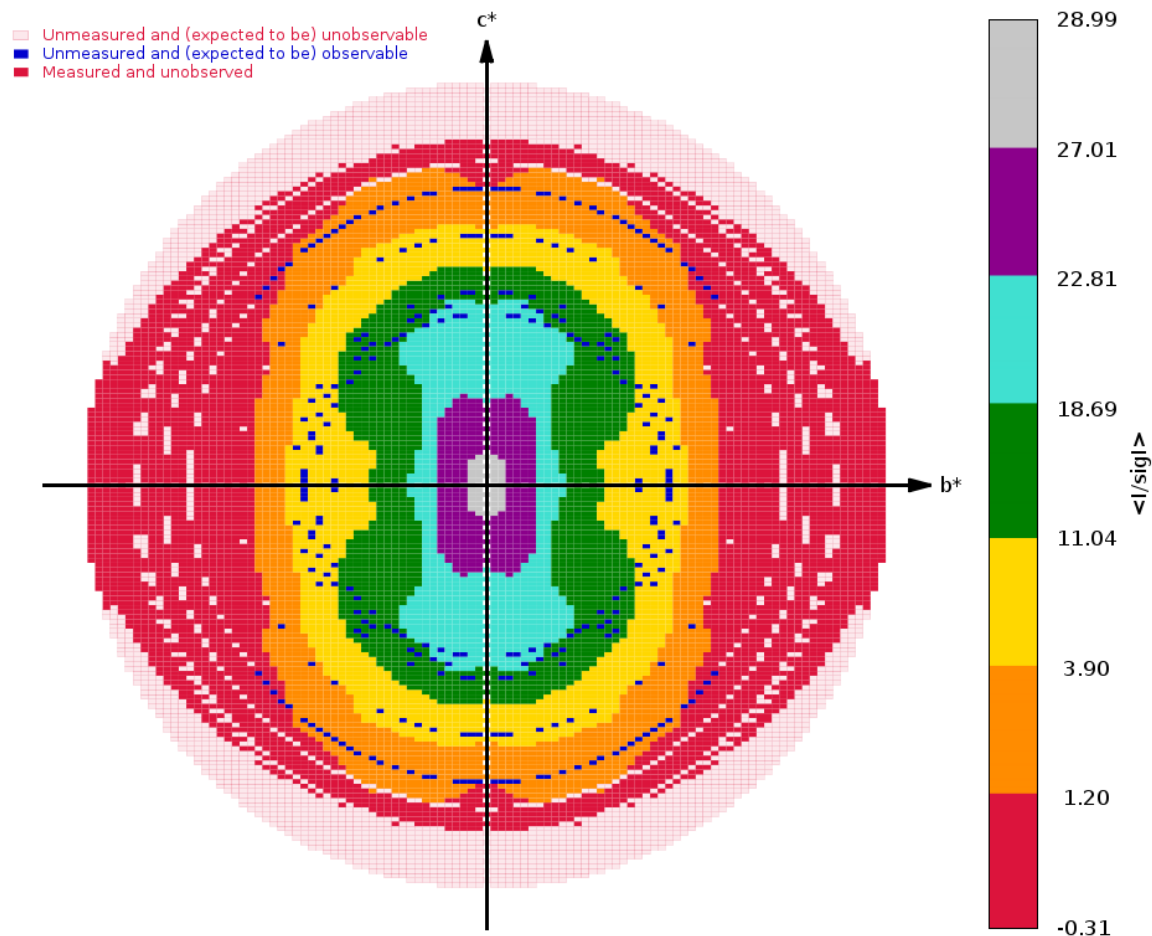
autoPROC: STARANISO plots



autoPROC: STARANISO plots

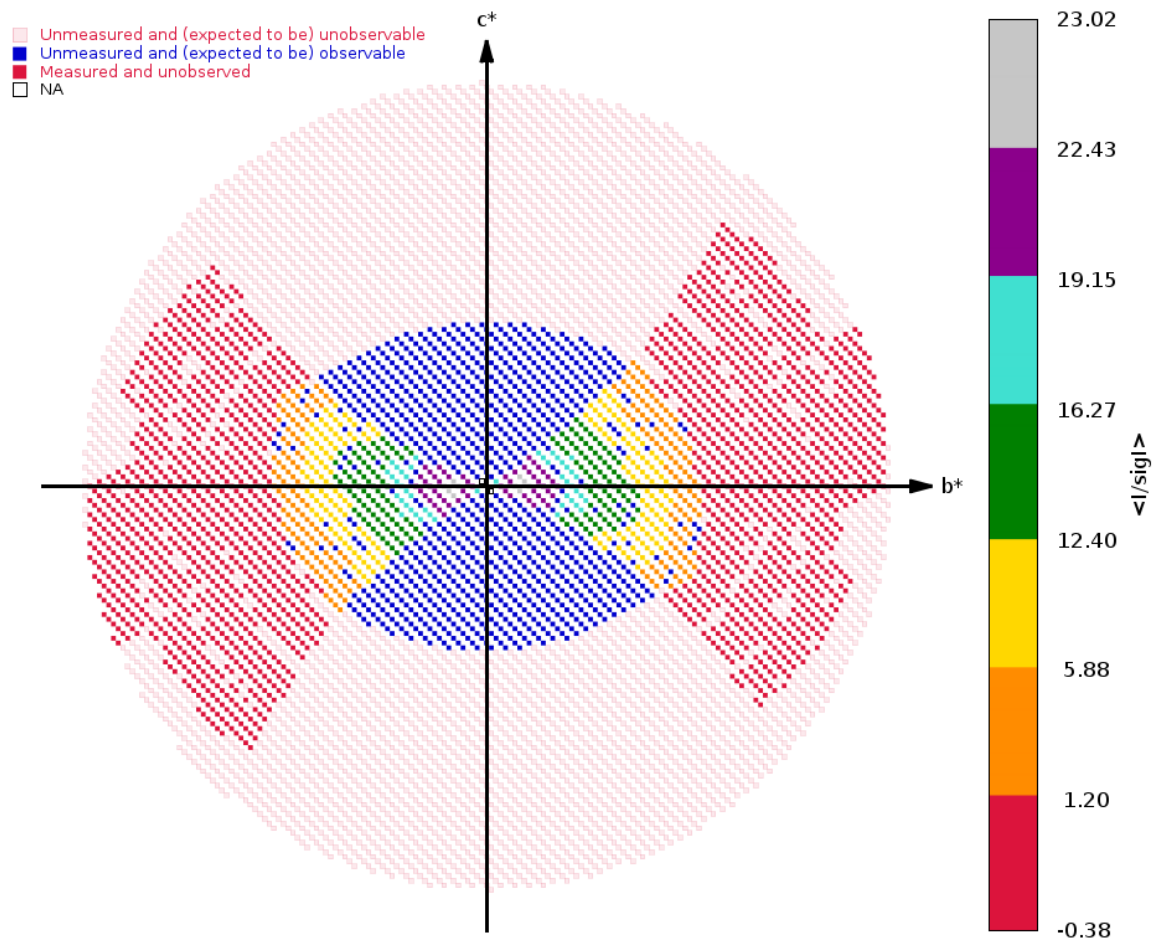
multi-sweep

ice-rings



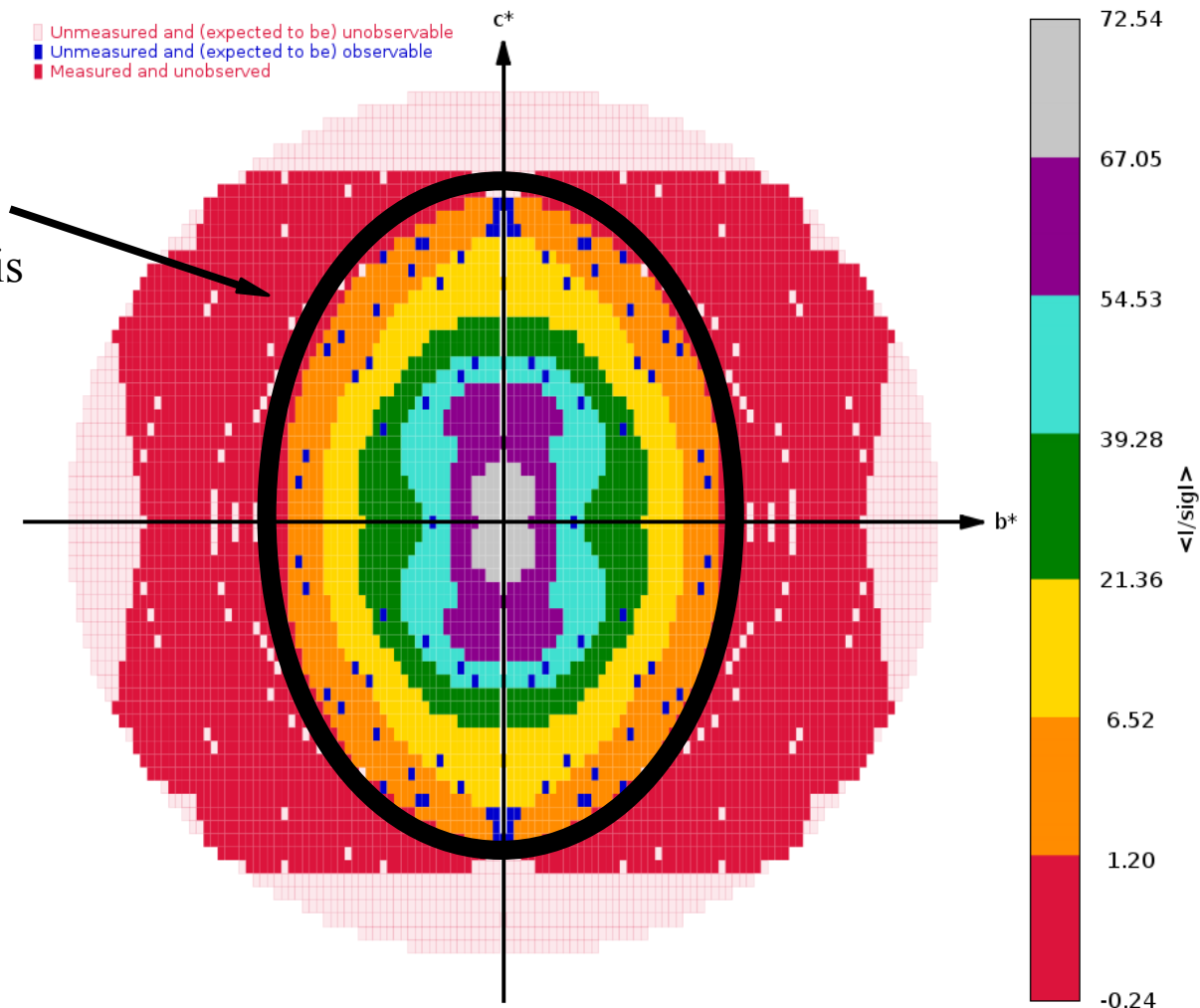
autoPROC: STARANISO plots

systematic
absences

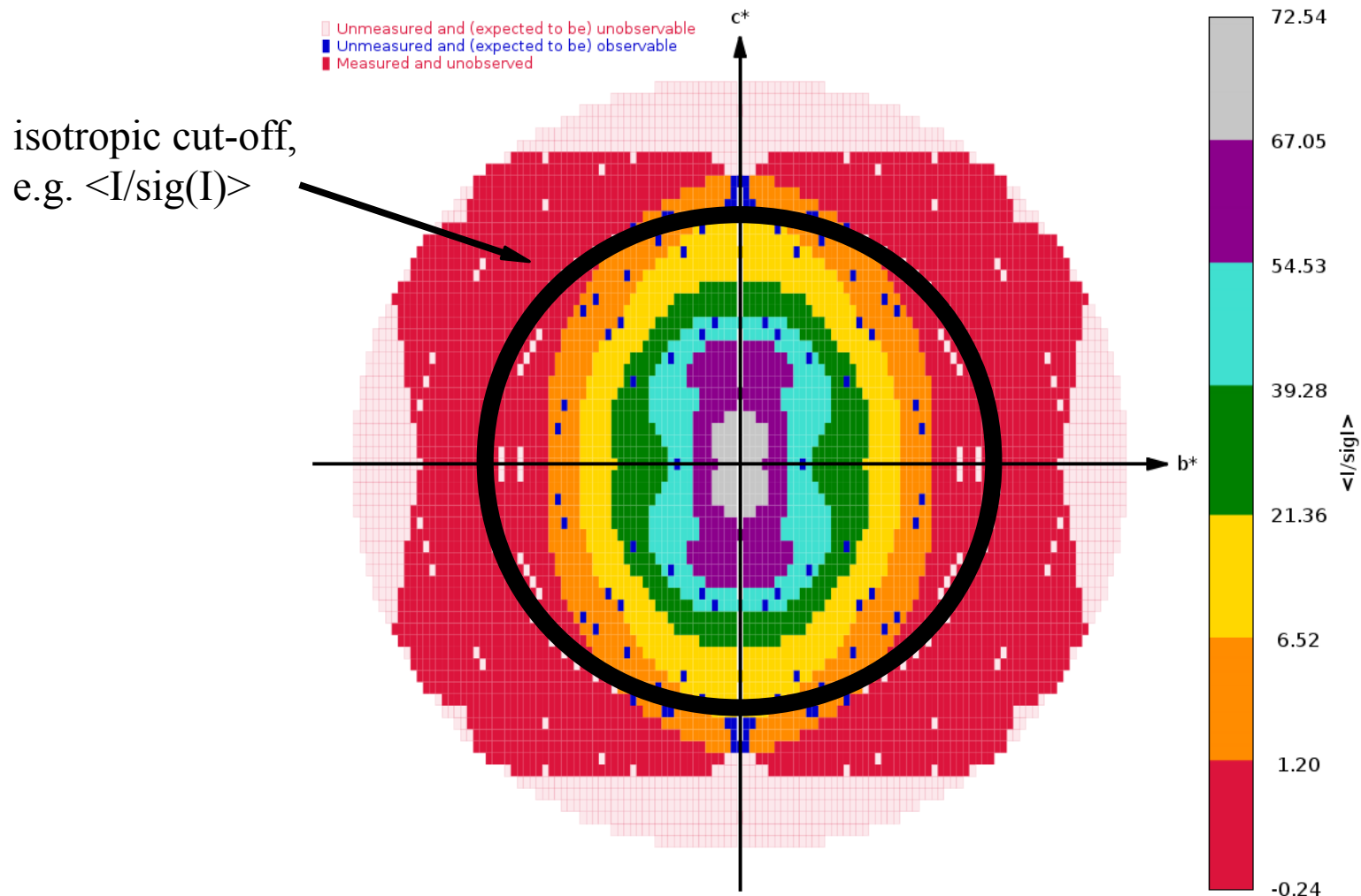


autoPROC: STARANISO plots

anisotropic cut-off
(fitted ellipsoid is *only* model and not used for cutting data!)



autoPROC: STARANISO plots



2.7. Finalising

Output file created (classical isotropic treatment of data) = [truncate-unique.mtz](#)

Spacegroup name	P21		
Unit cell parameters	50.68 89.80 60.47 90.000 94.778 90.000		
Wavelength	0.97940 Å		
	Overall	InnerShell	OuterShell
-----	-----	-----	-----
Low resolution limit	89.800	89.800	1.970
High resolution limit	1.937	5.258	1.937
Rmerge (all I+ & I-)	0.104	0.055	0.637
Rmerge (within I+/I-)	0.089	0.039	0.610
Rmeas (within I+/I-)	0.122	0.054	0.831
Rmeas (all I+ & I-)	0.124	0.066	0.751
Rpim (within I+/I-)	0.083	0.038	0.561
Rpim (all I+ & I-)	0.066	0.036	0.394
Total number of observations	127299	6404	6869
Total number unique	37680	1951	1947
Mean(I)/sd(I)	9.1	20.6	2.3
Completeness	93.8	94.1	98.0
Multiplicity	3.4	3.3	3.5
CC(1/2)	0.994	0.992	0.796
Anomalous completeness	83.2	84.2	86.3
Anomalous multiplicity	1.8	1.8	1.9
CC(ano)	0.121	0.479	0.090
DANO /sd(DANO)	0.890	1.402	0.772

autoPROC: “table 1” - anisotropic

Final output file created (including analysis of anisotropy via [STARANISO](#)) = [staraniso_alldata.mtz](#) (see above for detailed analysis of anisotropy)

```

Spacegroup name      P21
Unit cell parameters 50.68 89.80 60.47 90.000 94.778 90.000
Wavelength           0.97940 Å

Resolution limits & eigenvectors of ellipsoid fitted to resolution cut-off surface:
2.163      0.9996  0.0000  0.0279      0.998 _a_* - 0.066 _c_*
1.658      0.0000  1.0000  0.0000      _b_*
1.647      -0.0279  0.0000  0.9996     -0.023 _a_* + _c_*

-----
Overall  InnerShell  OuterShell
-----
Low resolution limit      89.800      89.800      1.761
High resolution limit     1.647       5.075      1.647

Rmerge (all I+ & I-)      0.108      0.055      0.911
Rmerge (within I+/I-)    0.093      0.039      1.034
Rmeas (within I+/I-)     0.127      0.054      1.290
Rmeas (all I+ & I-)      0.129      0.066      1.082
Rpim (within I+/I-)      0.085      0.038      0.766
Rpim (all I+ & I-)       0.069      0.035      0.576
Total number of observations 143816     7084      7292
Total number unique       43159      2150      2143
Mean(I)/sd(I)             8.2        20.5       1.5
Completeness (spherical)   66.2       94.3      18.2
Completeness (ellipsoidal) 86.7       94.3      58.3
Multiplicity              3.3        3.3       3.4
CC(1/2)                   0.994      0.992      0.476

Anomalous completeness (spherical) 56.1      84.7      13.1
Anomalous completeness (ellipsoidal) 73.5      84.7      39.5
Anomalous multiplicity          1.8        1.8       1.9
CC(ano)                        0.112      0.410     -0.130
|DANO|/sd(DANO)                0.895      1.375      0.889

```

- ❑ autoPROC needs to be general and generic enough to accommodate very different usage scenarios
- ❑ GPhL would like to have some control/input about what is presented and in what way:
 - This represents the “added value” provided by autoPROC compared to other data-processing pipelines (which have their own, distinct “added value”)
 - The common subset of results produced by different processing pipelines/programs will not necessarily provide the most value to users (lowest common denominator)
- ❑ How can GPhL help ISPyB (as deployed/used at synchrotrons) to extract and display the annotated results from autoPROC ... instead of each ISPyB site having to hunt around for files, tables and plots, trying to figure out what they mean and forgetting about others?
- ❑ Or maybe tools are already available and common to different sites?

1. Setup

1.1. Checking input

2. Processing dataset

2.1. Indexing

1 warning

2.2. Integration (initial)

1 warning

2.3. Post-refinement

2.4. Integration (further)

2.5. Scaling

2.6. Anisotropy analysis

2.7. Finalising



Global Phasing Limited

autoPROC 1.3.0 (20180117)

[autoPROC home page](#)[autoPROC Wiki](#)[autoPROC manual \(local copy\)](#)**Please cite:**

autoPROC : Vonrhein, C., Flensburg, C., Keller, P., Sharff, A., Smart, O., Paciorek, W., Womack, T. & Bricogne, G. (2011). Data processing and analysis with the autoPROC toolbox. Acta Cryst. D67, 293-302.

XDS : Kabsch, W. (2010). XDS. Acta Cryst. D66, 125-132.

POINTLESS : Evans, P.R. (2006). Scaling and assessment of data quality, Acta Cryst. D62, 72-82.

AIMLESS : Evans, P.R. & Murshudov, G.N. (2013). How good are my data and what is the resolution?, Acta Cryst. D69, 1204-1214.

CCP4 : Winn, M.D., Ballard, C.C., Cowtan, K.D., Dodson, E.J., Emsley, P., Evans, P.R., Keegan, R.M., Krissinel, E.B., Leslie, A.G.W., McCoy, A., McNicholas, S.J., Murshudov, G.N., Pannu, N.S., Potterton, E.A., Powell, H.R., Read, R.J., Vagin, A. & Wilson, K.S. (2011). Overview of the CCP4 suite and current developments, Acta. Cryst. D67, 235-242.

STARANISO : Tickle, I.J., Flensburg, C., Keller, P., Paciorek, W., Sharff, A., Vonrhein, C., & Bricogne, G. (2017). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.

Program versions used:

XDS : Nov 11, 2017 (BUILT 20171111)

POINTLESS : 1.11.8

AIMLESS : 0.6.1

CCP4 : 7.0.049

STARANISO : 1.10.9 (20171213)

1. Setup

```

Host      : babinet
OS        : DISTRI8_DESCRIPTION="Ubuntu 14.04.5 LTS"
           x86_64
           3.13.0-137-generic
User      : vonrhein (group = gphl)
Directory : /home/vonrhein/Projects/PanDDA/20180116/Results.babinet/NUDT21A-x0717
Date      : Wed Jan 17 09:41:04 GMT 2018
autoPROC  : /public/xtal/Server-nightly-alpha-bdg-linux64

```

Command-line arguments:

```
-nthreads 4 -l /home/vonrhein/Projects/PanDDA/20180116/Data/NUDT21A-x0717 -d 01
```

1.1. [Checking input](#)

ID	Directory	Files	Range
NUDT21A-x0717_1	/home/vonrhein/Projects/PanDDA/20180116/Data/NUDT21A-x0717	NUDT21A-x0717_1_####.cbf	1-1500

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2. Processing dataset**2.1. Indexing**

```
Header information from first image
(/home/vonrhein/Projects/PanDDA/20180116/Data/NUDT21A-x0717/NUDT21A-x0717_1_0001.cbf):
date                        = 08 Jul 2017 07:10:42.124
exposure time               [seconds] = 0.037
distance                    [mm]      = 275.210
wavelength                  [Å]       = 0.928190
Phi-angle                   [degree]  = 0.00000
Omega-angle (start, end)   [degree]  = 72.00000 72.12000
Oscillation-angle in Omega [degree]  = 0.12000
Kappa-angle                 [degree]  = 0.00000
2-Theta angle              [degree]  = 0.00000
Beam centre in X            [pixel]   = 1235.280
Beam centre in Y            [pixel]   = 1458.870
```

Using spots from images 1-1500

Goniostat angles for first image are Omega,Kappa,Phi = 72.000,0.000,0.000

Indexing solution with largest number of indexed spots = Lattice01



Click for more information/plots

(minimum) angle between orientations for Lattice01 (18855 spots) and Lattice02 (11597 spots) - assuming space group P1 = 179.7 degree

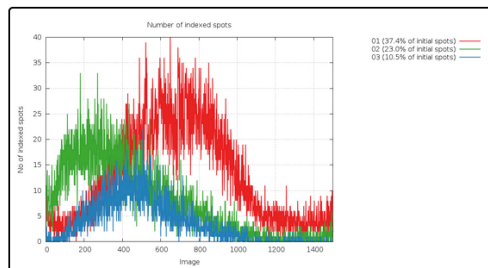


Click for more information/plots

(minimum) angle between orientations for Lattice01 (18855 spots) and Lattice03 (5280 spots) - assuming space group P1 = 120.3 degree



Click for more information/plots

Number of spots for each significant indexing solution (as a function of image number) ([explanation](#))Picking indexing solution that used the most spots (=O1) - for details see [run_idxref.log](#)

Indexing used 37% of the initial 50476 events

1. Setup

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Indexing uses 37% of the initial 50476 spots

WARNING

The selected indexing solution uses less than 50% of initial spots - please check this carefully for ice-rings, multiple lattices or problematic spot searching (due to poor initial background estimation).

Automatically added 2 EXCLUDE_RESOLUTION_RANGE cards (to accommodate possible ice-rings) - based on automatic analysis (see [xds_spots2res.log](#) for details). If you don't want this behaviour, please set `XdsExcludeIceRingsAutomatically="no"` on the command-line.

Based on analysis of indexed spots we would recommend a low-resolution limit of 50.00 Å. You can set this on the command-line (e.g. adding `reslow=50.00`).

Based on all indexed spots, a high-resolution limit of at least 2.51 Å should be possible.

```
SPACE GROUP AND CELL PARAMETERS ARE UNKNOWN
AUTOINDEXING IS BASED ON 18861 OUT OF 18861 SPOTS

***** INDEXING OF OBSERVED SPOTS IN SPACE GROUP # 1 *****
18774 OUT OF 18861 SPOTS INDEXED.
7 REJECTED REFLECTIONS (REASON: OVERLAP)
80 REJECTED REFLECTIONS (REASON: TOO FAR FROM IDEAL POSITION)
EXPECTED ERROR IN SPINDLE POSITION 0.409 DEGREES
EXPECTED ERROR IN DETECTOR POSITION 0.64 PIXELS

***** DIFFRACTION PARAMETERS USED AT START OF INTEGRATION *****

REFINED VALUES OF DIFFRACTION PARAMETERS DERIVED FROM 18774 INDEXED SPOTS
REFINED PARAMETERS: BEAM ORIENTATION CELL AXIS
STANDARD DEVIATION OF SPOT POSITION (PIXELS) 0.63
STANDARD DEVIATION OF SPINDLE POSITION (DEGREES) 0.41
SPACE GROUP NUMBER 1
UNIT CELL PARAMETERS 59.934 59.955 215.885 89.997 89.946 60.164
REC. CELL PARAMETERS 0.019235 0.019228 0.004632 89.972 90.061 119.836
COORDINATES OF UNIT CELL A-AXIS -53.429 -11.971 24.374
COORDINATES OF UNIT CELL B-AXIS -49.780 22.461 -24.740
COORDINATES OF UNIT CELL C-AXIS -17.540 -175.684 -124.233
CRYSTAL MOSAICITY (DEGREES) 0.200
LAB COORDINATES OF ROTATION AXIS 0.999996 -0.000628 0.002587
DIRECT BEAM COORDINATES (REC. ANGSTROM) 0.000732 0.000499 1.077365
DETECTOR COORDINATES (PIXELS) OF DIRECT BEAM 1236.37 1459.61
DETECTOR ORIGIN (PIXELS) AT 1235.28 1458.87
CRYSTAL TO DETECTOR DISTANCE (mm) 275.21
LAB COORDINATES OF DETECTOR X-AXIS 1.000000 0.000000 0.000000
LAB COORDINATES OF DETECTOR Y-AXIS 0.000000 1.000000 0.000000
```

LATTICE- CHARACTER	BRAVAIS- LATTICE	QUALITY OF FIT	UNIT CELL CONSTANTS (ANGSTROM & DEGREES)					
			a	b	c	alpha	beta	gamma
31	aP	0.0	59.9	60.0	215.9	90.0	89.9	60.2
44	aP	0.1	59.9	60.0	215.9	90.0	90.1	119.8
39	mC	1.8	104.0	60.0	215.9	90.0	90.1	89.8
34	mP	1.9	59.9	215.9	60.0	90.0	119.8	90.1
29	mC	1.9	59.9	104.0	215.9	90.0	90.1	89.8
10	mC	2.0	103.7	60.1	215.9	90.1	90.0	90.0
13	oC	2.2	60.1	103.7	215.9	90.0	90.1	90.0

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10	mC	2.0	103.7	60.1	215.9	90.1	90.0	90.0
13	oC	2.2	60.1	103.7	215.9	90.0	90.1	90.0
14	mC	2.2	60.1	103.7	215.9	90.0	90.1	90.0
38	oC	3.0	59.9	104.0	215.9	90.0	90.1	90.2
12	hP	3.4	59.9	60.0	215.9	90.0	90.1	119.8
33	mP	249.0	59.9	60.0	215.9	90.0	90.1	119.8
35	mP	249.4	59.9	60.0	215.9	90.0	90.1	119.8

BRAVAIS-

TYPE

aP

mP

mC, mI

oC

hP

POSSIBLE SPACE-GROUPS FOR PROTEIN CRYSTALS

[SPACE GROUP NUMBER, SYMBOL]

[1, P1]

[3, P2] [4, P2(1)]

[5, C2]

[21, C222] [20, C222(1)]

[143, P3] [144, P3(1)] [145, P3(2)] [149, P312] [150, P321] [151, P3(1)12]

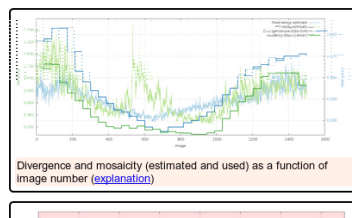
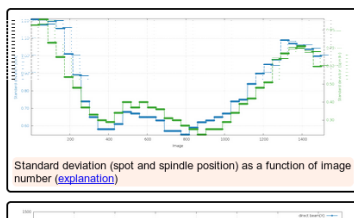
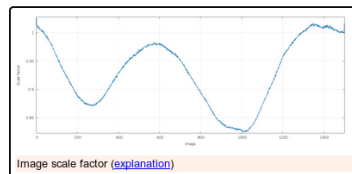
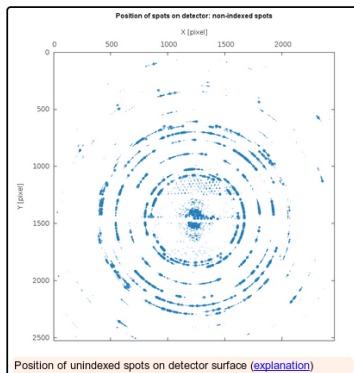
[152, P3(1)21] [153, P3(2)12] [154, P3(2)21] [168, P6] [169, P6(1)]

[170, P6(5)] [171, P6(2)] [172, P6(4)] [173, P6(3)] [177, P622]

[178, P6(1)22] [179, P6(5)22] [180, P6(2)22] [181, P6(4)22] [182, P6(3)22]

Click for more information/plots

2.2. Integration (initial)



1. Setup

1.1. Checking input

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1 warning

2.2. Integration (initial)

1 warning

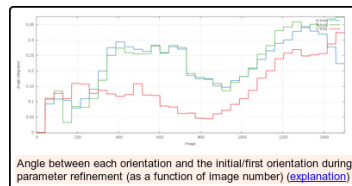
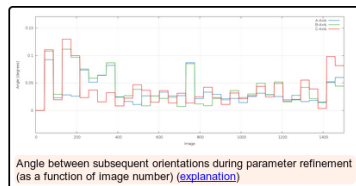
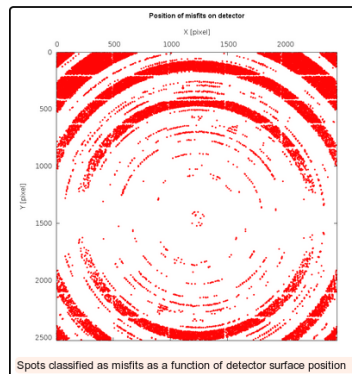
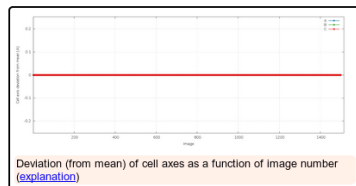
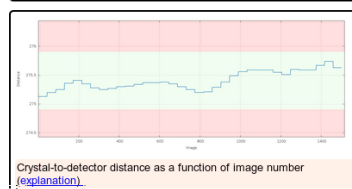
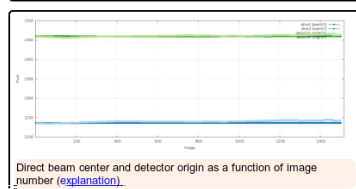
2.3. Post-refinement

2.4. Integration (further)

2.5. Scaling

2.6. Anisotropy analysis

2.7. Finalising



WARNING

Distance refinement seems unstable: the refined distance deviates from the mean value of 275.41 mm by $\pm 0.33/0.28$ mm.

2.3. Post-refinement

Analysis of data with POINTLESS

Scores for each symmetry element

1. Setup

1.1. Checking input

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2.1. Indexing

1 warning

2.2. Integration (initial)

1 warning

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Scores for each symmetry element

Nelmt	Lklhd	Z-cc	CC	N	Rmeas	Symmetry & operator (in Lattice Cell)
1	0.883	9.19	0.92	42417	0.100	identity
2	0.060	1.58	0.16	85919	0.836	2-fold l (0 0 1) {-h,-k,l}
3	0.061	1.62	0.16	79831	0.824	2-fold k (0 1 0) {-h,h+k,-l}
4	0.061	1.65	0.16	81405	0.817	2-fold h (1 0 0) {h+k,-k,-l}
5	0.062	1.72	0.17	88265	0.828	2-fold (1-1 0) {-k,-h,-l}
6	0.903	8.78	0.88	83014	0.142	2-fold (2-1 0) {h,-h-k,-l}
7	0.917	8.28	0.83	79611	0.167	2-fold (-1 2 0) {-h-k,k,-l}
8	0.917	8.27	0.83	86342	0.176	2-fold (1 1 0) {k,h,-l}
9	0.916	8.15	0.82	162967	0.192	3-fold l (0 0 1) {k,-h-k,l}{-h-k,h,l}
10	0.061	1.61	0.16	166246	0.819	6-fold l (0 0 1) {h+k,-h,l}{-k,h+k,l}

Best Solution: space group P 31 2 1

Reindex operator: [-h,k,-l]
 Laue group probability: 0.996
 Systematic absence probability: 0.820
 Total probability: 0.817
 Space group confidence: 0.722
 Laue group confidence: 0.996

WARNING: You will have to resolve the enantiomorphic ambiguity later

Unit cell: 59.92 59.92 215.93 90.00 89.96 119.87

Some initial processing statistics

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	R-FACTOR COMPARED	1/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano
3.30	46872	11584	13084	88.5%	5.4%	4.8%	46311	24.28	6.2%	99.6*	44*	1.284	4379
2.33	79012	20019	23018	84.0%	18.1%	16.5%	77660	8.10	20.7%	98.7*	15*	0.973	7305
1.91	86747	22945	30836	74.4%	86.2%	74.2%	84006	1.83	91.7%	82.9*	17*	0.804	7903
1.65	114128	30497	36426	83.7%	409.0%	447.3%	109957	0.30	467.9%	19.2*	2	0.574	10627
1.48	108623	32496	41451	78.4%	8815.3%	9673.9%	104573	0.00	18335.8%	50.4*	5	0.509	10317
1.35	89600	32346	45736	70.7%	-99.9%	-99.9%	84530	0.00	-99.9%	5.0	4	0.401	9404
1.25	66943	30285	49491	61.2%	-99.9%	-99.9%	57132	0.00	-99.9%	11.6*	5	0.481	7867
1.17	25607	19579	53545	36.6%	-99.9%	-99.9%	11460	0.00	-99.9%	3.8	3	0.463	1516
1.10	7158	6674	56077	11.7%	3311.9%	3785.9%	968	0.00	4603.7%	1.1	-3	0.518	76
total	624690	206425	351264	58.8%	22.6%	22.7%	576677	2.40	26.5%	99.5*	13*	0.677	58954

a b Isa (see Diederichs, Acta Cryst. (2010). D66, 733-740)
 8.688E-01 3.410E-03 18.37

There are consistent indications of anomalous signal in [CORRECTLP](#) and [CORRECT_ana_ano_all.mrfana](#). Data completeness (0.627) and multiplicity (5.0) seem sufficiently high to give those indications some reliability.

2.4. Integration (further)**Processing statistics**

RESOLUTION LIMIT	NUMBER OF REFLECTIONS OBSERVED	UNIQUE	POSSIBLE	COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	R-FACTOR COMPARED	1/SIGMA	R-meas	CC(1/2)	Anomal Corr	SigAno	Nano
3.30	54182	12641	13038	97.0%	6.4%	5.3%	53869	23.89	7.4%	99.6*	58*	1.535	5188
2.34	90246	21611	23766	90.9%	22.2%	19.0%	88649	7.53	25.3%	98.1*	28*	1.058	8151
1.91	97525	24393	30780	79.5%	92.3%	88.0%	94960	1.79	104.9%	83.8*	20*	0.864	8783
1.65	124295	32153	36386	88.4%	435.4%	486.5%	120806	0.28	496.1%	16.7*	2	0.564	11024
1.48	119140	34480	41341	83.4%	36702.8%	41112.5%	114656	0.00	47272.6%	9.3	4	0.498	11191
1.35	98020	34263	45540	75.2%	-99.9%	-99.9%	92571	0.00	-99.9%	13.7*	2	0.475	10522
1.25	73868	32674	49503	66.0%	-99.9%	-99.9%	63647	0.00	-99.9%	12.4*	5	0.479	8877
1.17	20350	21143	53315	39.7%	-99.9%	-99.9%	13525	0.00	-99.9%	3.2	3	0.454	2005
1.10	8143	7422	56691	13.1%	1816.5%	2183.4%	1442	0.01	2568.9%	4.2	2	0.441	145

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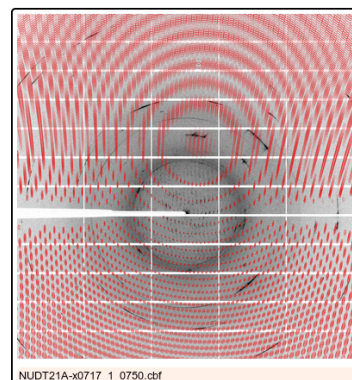
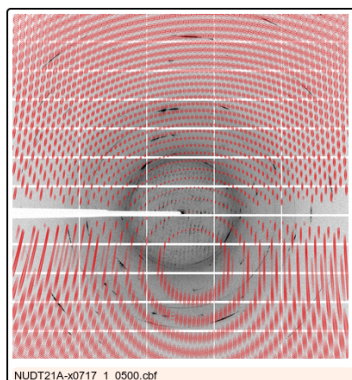
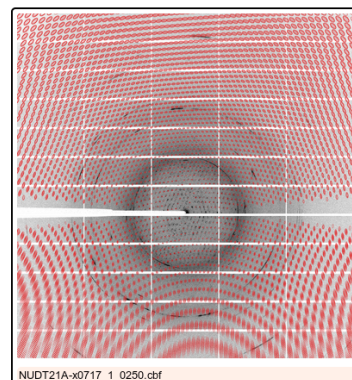
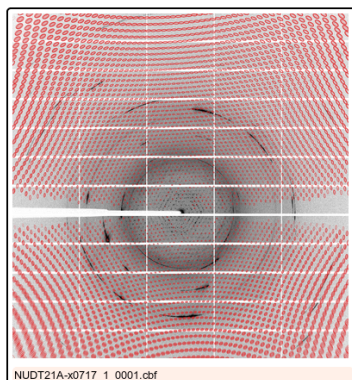
1.25	73808	32674	49583	66.0%	-99.9%	-99.9%	63647	0.00	-99.9%	12.4*	5	0.479	8877
1.17	28350	21143	53315	39.7%	-99.9%	-99.9%	13525	0.00	-99.9%	3.2*	3	0.454	2085
1.10	8143	7422	56691	13.1%	1816.5%	2183.4%	1442	0.01	2568.9%	4.2	2	0.441	145
total	693769	220780	350288	63.0%	25.2%	25.2%	643325	2.33	29.3%	99.4*	20*	0.701	65966

a b Isa (see Diederichs, Acta Cryst. (2010). D66, 733-740)

8.791E-01 3.125E-03 19.08

8 overloaded reflections out of 719530 total

Click for more information plots



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[staraniso_alldata.mtz](#)

2.6. Anisotropy analysis

STARANISO analyses merged intensity data for [anisotropy](#) of diffraction, applies an anisotropic cut-off as well as a correction and finally performs Bayesian estimation of structure amplitudes. See also [STARANISO server](#) and [program details](#).

Resolution limits & eigenvectors of ellipsoid fitted to resolution cut-off surface:

2.142	1.0000	0.0000	0.0000	0.894 _a_* - 0.447 _b_*
2.142	0.0000	1.0000	0.0000	_b_*
1.706	0.0000	0.0000	1.0000	_c_*

Lowest cut-off resolution limit:
2.587 at reflection 20 0 -6 in direction 0.958 _a_* - 0.287 _c_*

Worst resolution limit after cut-off:
3.241 at reflection 16 0 -1 in direction 0.998 _a_* - 0.062 _c_*

Best resolution limit after cut-off:
1.719 at reflection 4 3 123 in direction 0.032 _a_* + 0.024 _b_* + 0.999 _c_*

Because the cut-off surface is likely to be only very approximately ellipsoidal, in part due to variations in reflection redundancy arising from the chosen collection strategy, the directions of the worst and best resolution limits may not correspond with the reciprocal axes, even in high-symmetry space groups (the only constraint being that the surface must have point symmetry at least that of the Laue class).

Fraction of data inside cut-off surface: 23.5% (29014 / 123476)

Fraction of cut-off surface above threshold: 5.7% (115 / 2032)

Scale: 1.492E+00 [= factor to place Iobs on same scale as Iprofile/100.]
Beq: 29.18 [= equivalent overall isotropic B factor on Fs.]

Delta-B tensor:

B11	B22	B33
5.11	5.11	-10.22

The delta-B tensor is the overall anisotropy tensor on Fs after subtraction of Beq from its diagonal elements (so trace = 0).

Eigenvalues (E) & eigenvectors of overall anisotropy (B) tensor on Fs:

34.30	1.0000	0.0000	0.0000	0.894 _a_* - 0.447 _b_*
34.30	0.0000	1.0000	0.0000	_b_*
18.96	0.0000	0.0000	1.0000	_c_*

The eigenvalues and eigenvectors of the overall B tensor are the squares of the lengths and the directions of the principal axes of the ellipsoid that represents the tensor.

Delta-B eigenvalues: 5.11 5.11 -10.22

The delta-B eigenvalues are the eigenvalues of the overall anisotropy tensor after subtraction of Beq (so sum = 0).

Anisotropy ratio: 0.526 [= (Emax - Emin) / Beq]
Fractional anisotropy: 0.295 [= sqrt(1.5 Sum i (E i - Beq)^2 / Sum i E i^2)]
Anisotropic S/N ratio: 9.70 [= max_h | exp(4 pi^2 s_-h delta(B) s_h) - 1 | < I_h/sd(I_h) >]

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Anisotropic S/N ratio: 9.70 $[= \max_h | \exp(4 \pi^2 s_h \Delta(B) s_h) - 1 | < I_h / \sigma(I_h) >]$

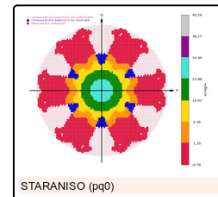
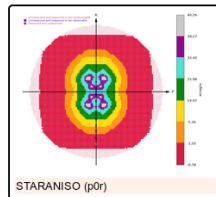
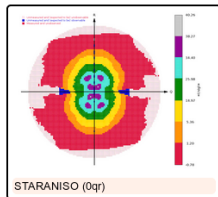
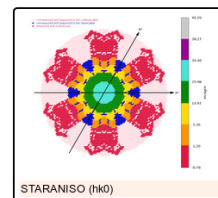
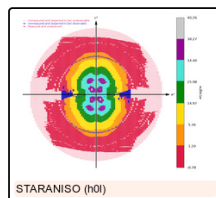
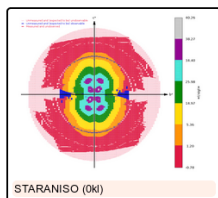
The 'anisotropic S/N ratio', unlike the 'anisotropy ratio' or the 'fractional anisotropy' shown above, in addition to the anisotropy of the B tensor, takes both the resolution and the local mean $I/\sigma(I)$ into account.

Output file created after STARANISO analysis of anisotropy = [staraniso_alldata.sca](#). This contains intensities (after applying an anisotropic high-resolution cut-off and correction) and can be used e.g. for experimental phasing with autoSHARP.

Output file created after STARANISO analysis of anisotropy = [staraniso_alldata.mtz](#). This contains intensities and amplitudes (after applying an anisotropic high-resolution cut-off and correction) and can be used for all subsequent stages, e.g. refinement in BUSTER.

For details see [staraniso_alldata.log](#)

Reciprocal plane plots generated from STARANISO analysis - see below.

**2.7. Finalising**

Output file created (classical isotropic treatment of data) = [truncate-unique.mtz](#) - see also [table1_stats.xml](#)

Spacegroup name	P3121		
Unit cell parameters	59.891 59.891 215.912 90.0 90.0 120.0		
Wavelength	0.92819 Å		
	Overall	InnerShell	OuterShell
Low resolution limit	51.867	51.867	2.176
High resolution limit	2.139	5.804	2.139
Rmerge (all I+ & I-)	0.143	0.057	1.327
Rmerge (with in T _h /T ₋)	0.135	0.051	1.267

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Mean(I)/sd(I)	12.5	30.4	2.8
Completeness	97.5	99.7	95.7
Multiplicity	7.3	7.2	7.6
CC(1/2)	0.994	0.999	0.703
Anomalous completeness	85.7	96.8	85.4
Anomalous multiplicity	4.3	4.3	4.3
CC(ano)	0.584	0.588	0.256
DANO /sd(DANO)	1.017	1.636	0.855

Final output file created (including analysis of anisotropy via [STARANISO](#)) = [staraniso_alldata-unique.mtz](#) (see above for detailed analysis of anisotropy) - see also [table1 stats.xml](#)

```

Spacegroup name      P3121
Unit cell parameters 59.891 59.891 215.912 90.0 90.0 120.0
Wavelength           0.92819 Å

Resolution limits & eigenvectors of ellipsoid fitted to resolution cut-off surface:
2.142    1.0000  0.0000  0.0000    0.894 _a_* - 0.447 _b_*
2.142    0.0000  1.0000  0.0000    _b_*
1.706    0.0000  0.0000  1.0000    _c_*

-----
Overall  InnerShell  OuterShell
-----
Low resolution limit      51.867      51.867      1.940
High resolution limit     1.723       5.800      1.723

Rmerge  (all I+ & I-)      0.172      0.057      1.606
Rmerge  (within I+/I-)     0.166      0.051      1.629
Rmeas   (all I+ & I-)      0.185      0.062      1.703
Rmeas   (within I+/I-)     0.189      0.058      1.823
Rpm     (all I+ & I-)      0.066      0.023      0.559
Rpm     (within I+/I-)     0.089      0.028      0.813
Total number of observations 226954    10388     12979
Total number unique         29013     1451      1450
Mean(I)/sd(I)              11.2       30.3       1.6
Completeness (spherical)    59.6      99.7      10.1
Completeness (ellipsoidal)  89.7      99.7      69.1
Multiplicity                7.8        7.2       9.0
CC(1/2)                    0.994      0.999     0.662

Anomalous completeness (spherical)  52.6      96.8       8.8
Anomalous completeness (ellipsoidal) 81.9      96.8      68.0
Anomalous multiplicity              4.5       4.3       5.0
CC(ano)                            0.552     0.505     0.029
|DANO|/sd(DANO)                    0.992     1.639     0.709

```

XML file written as [01/autoPROC.xml](#)

XML file written as [01/autoPROC_staraniso.xml](#) (for /home/vonrhein/Projects/PanDDA/20180116/Results.babinet/NUDT21A-x0717/01/staraniso_alldata-unique.mtz)

Summary of process output also created as HTML. Please point your browser to "file:///home/vonrhein/Projects/PanDDA/20180116/Results.babinet/NUDT21A-x0717/01/summary.html".

Elapsed time = 4205 seconds