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autoPROC 1.3.0 (20200318)
XDS VERSION Jan 31, 2020 BUILT=20200131
AIMLESS Version 0.7.4
STARANISO Version 2.3.33 (11-Apr-2020)
CCP4 Version 7.0.078
Host server8
User vonrhein (group = users)
Date Tue Apr 21 22:11:07 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
2a m1a2peg-2_#####.cbf (300 images, 150°)
3a m1a2peg-3_#####.cbf (350 images, 175°)
    
```

Isotropic data analysis:

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Spacegroup P1
Cell parameters 30.1468 37.7807 64.8130
                95.8014 97.9852 90.1138
Wavelength [Å] 0.97918
    
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	Overall	Inner Shell	Outer Shell
Low resolution limit	37.582	37.582	1.645
High resolution limit	1.617	4.386	1.617
Rmerge (all I+ & I-)	0.098	0.040	0.502
Rmeas (all I+ & I-)	0.125	0.053	0.710
Rpim (all I+ & I-)	0.075	0.034	0.502
Total number of observations	84195	3890	1703
Total number unique	31282	1648	1071
Mean(I)/sd(I)	18.2	39.5	5.3
Completeness	86.8	91.6	59.8
Multiplicity	2.7	2.4	1.6
CC(1/2)	0.990	0.992	0.481
Anomalous completeness	72.8	81.3	30.7
Anomalous multiplicity	1.5	1.2	1.0
CC(ano)	-0.072	0.135	NA
DANO /sd(DANO)	0.966	0.888	1.466

Final scaling/merging - isotropic data analysis

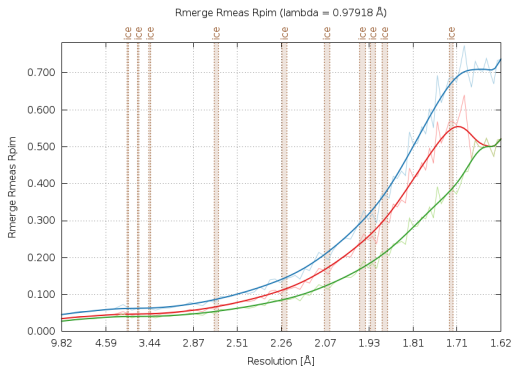


Fig.1 : R-values as a function of resolution

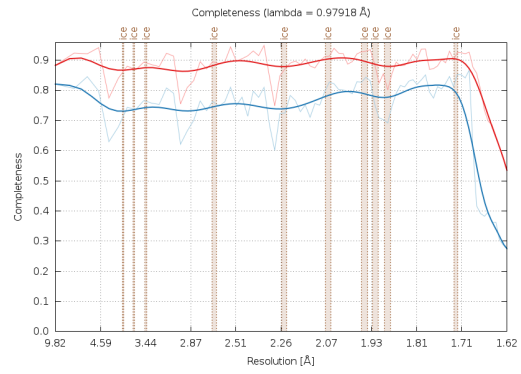


Fig.2 : Completeness as a function of resolution

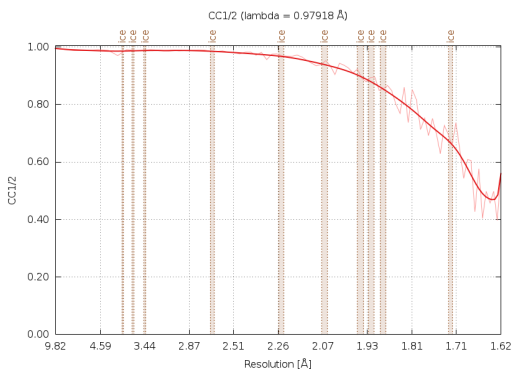


Fig.3 : CC1/2 as a function of resolution

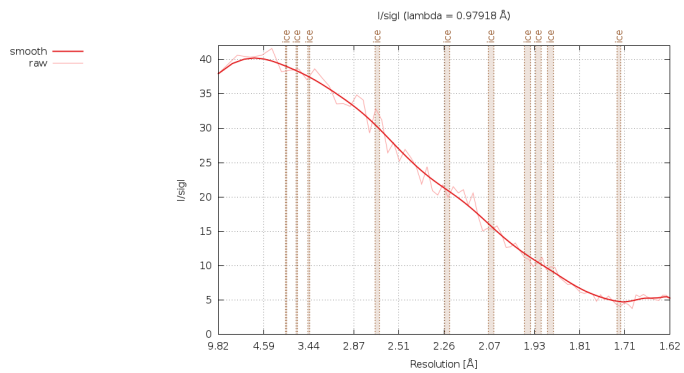


Fig.4 : I/sigI as a function of resolution

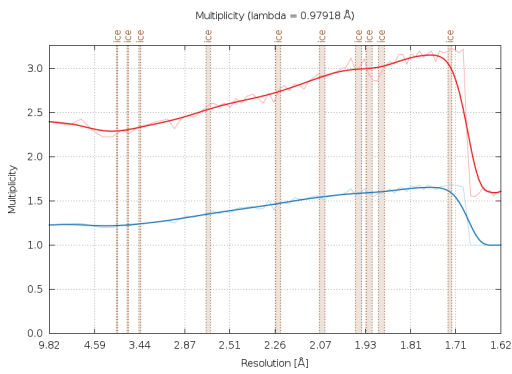


Fig.5 : Multiplicity as a function of resolution

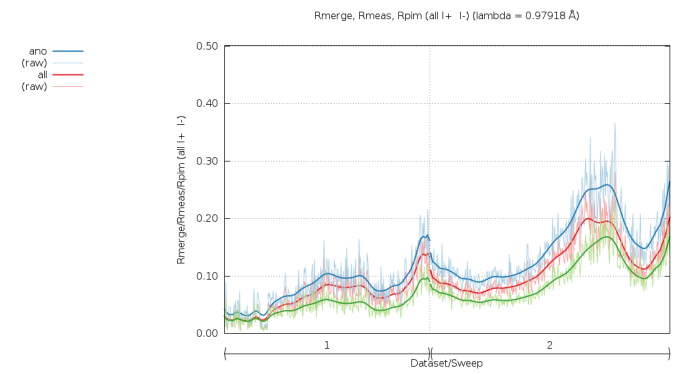


Fig.6 : R-values as a function of image number

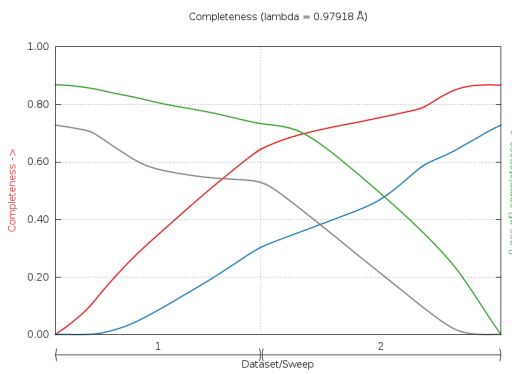


Fig.7 : Completeness as a function of image number

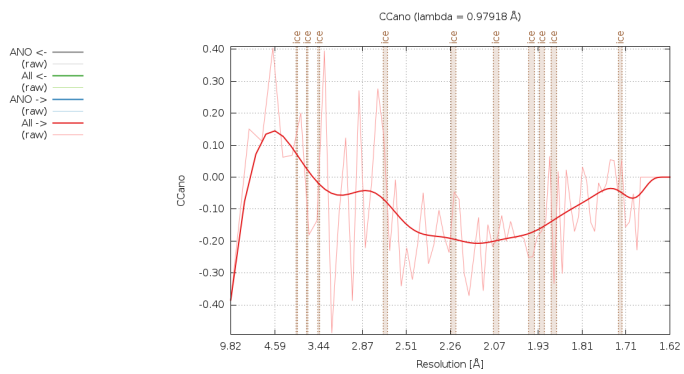


Fig.8 : CCano as a function of resolution

Final scaling/merging - isotropic data analysis

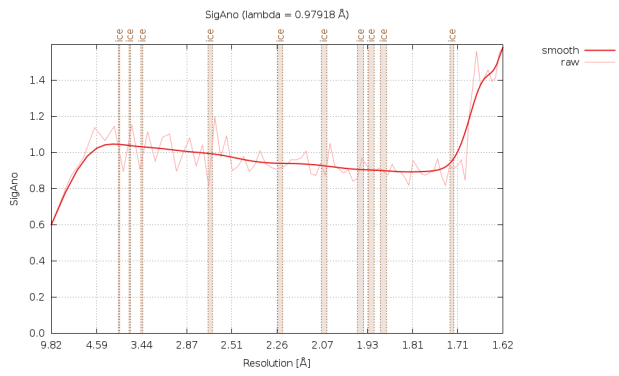


Fig.9 : SigAno as a function of resolution

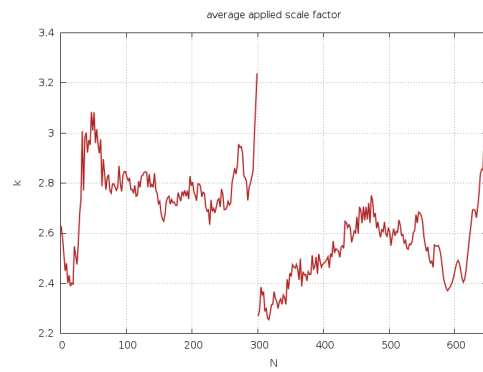


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

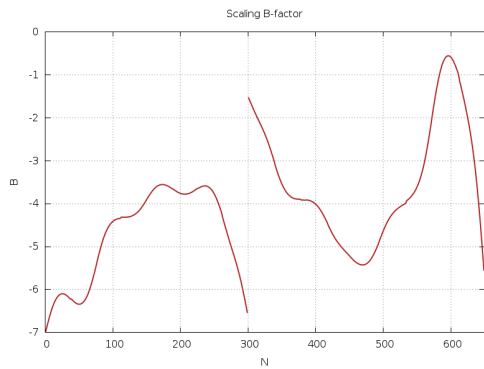


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

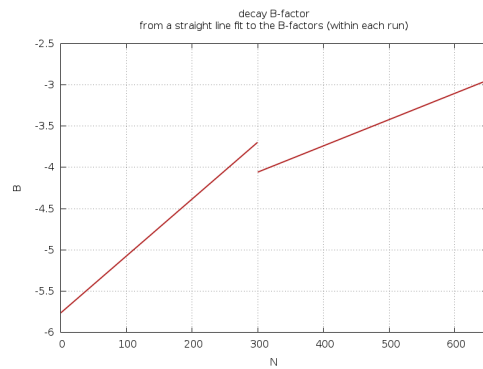


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

Data processing sweep 2a

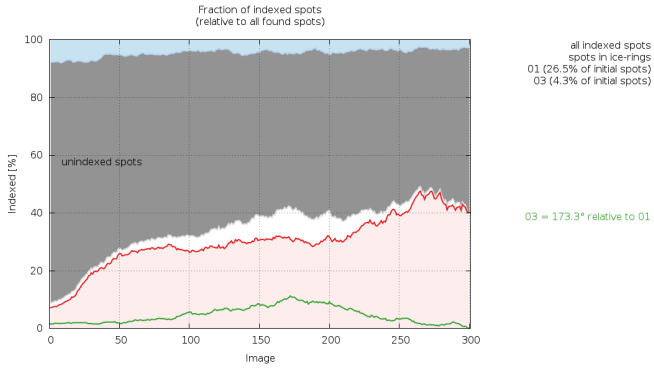


Fig.13 : (sweep 2a) number of spots for each indexing solution as a function of image number

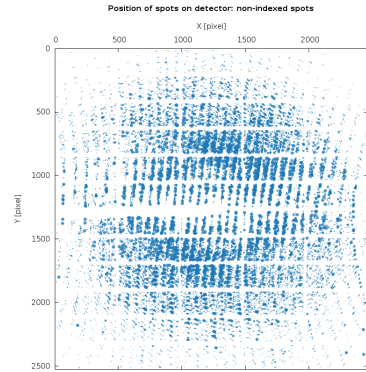


Fig.14 : (sweep 2a) unindexed spots as a function of detector position

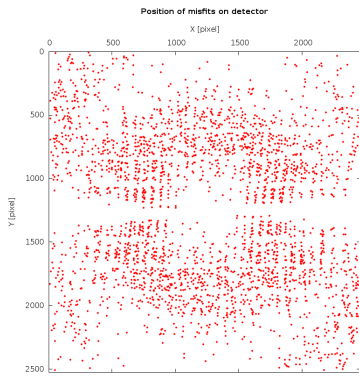


Fig.15 : (sweep 2a) reflections classified as misfits (as a function of detector position)

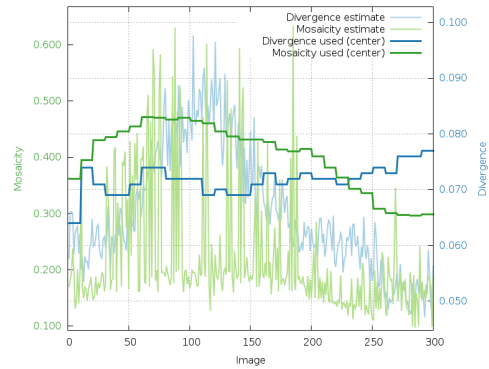


Fig.16 : (sweep 2a) divergence and mosaicity (estimated and used) as a function of image number

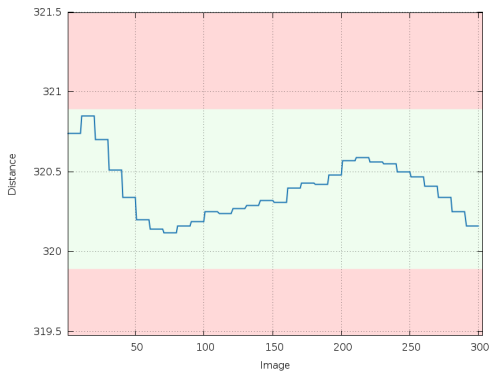


Fig.17 : (sweep 2a) refined crystal-to-detector distance as a function of image number

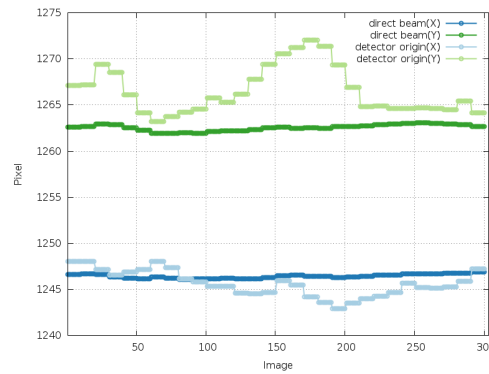


Fig.18 : (sweep 2a) direct beam position and detector origin as a function of image number

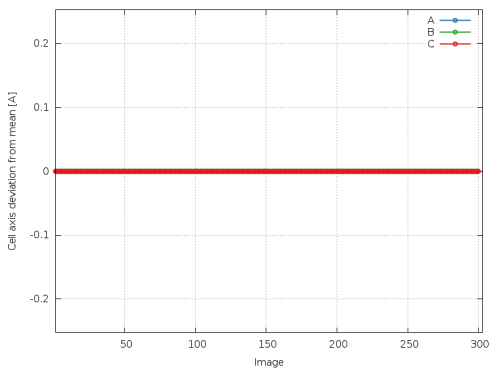


Fig.19 : (sweep 2a) deviation of refined cell axes relative to their mean (as a function of image number)

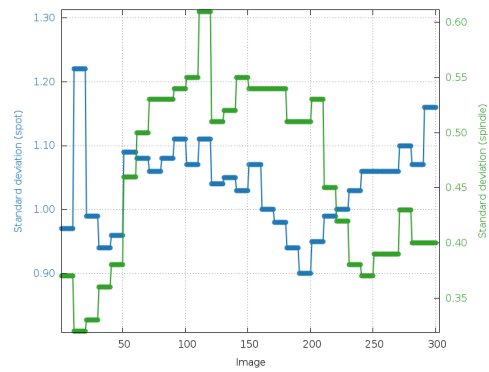


Fig.20 : (sweep 2a) standard deviation (spot position and spindle) as a function of image number

Data processing sweep 3a

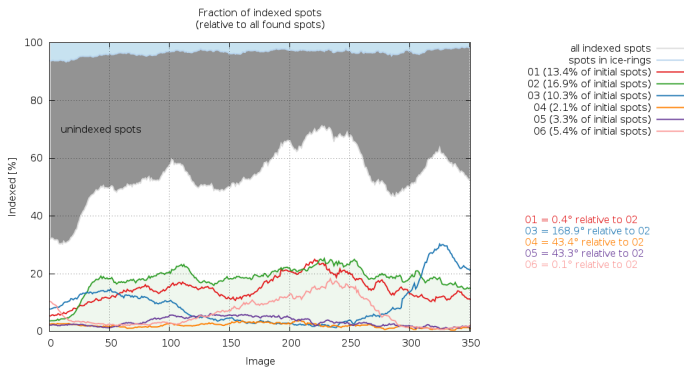


Fig.21 : (sweep 3a) number of spots for each indexing solution as a function of image number

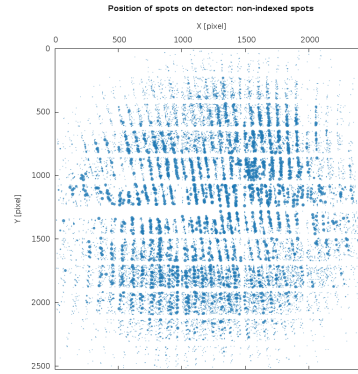


Fig.22 : (sweep 3a) unindexed spots as a function of detector position

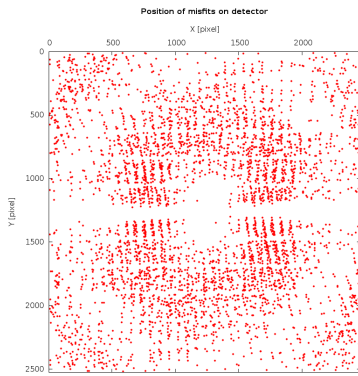


Fig.23 : (sweep 3a) reflections classified as misfits (as a function of detector position)

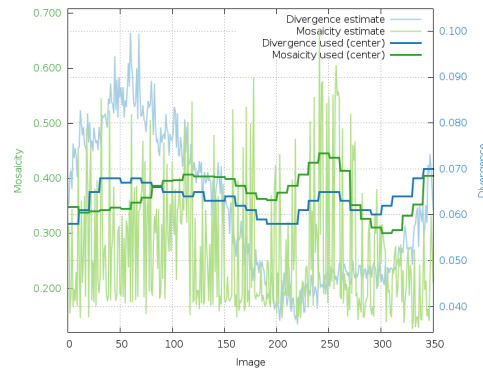


Fig.24 : (sweep 3a) divergence and mosaicity (estimated and used) as a function of image number

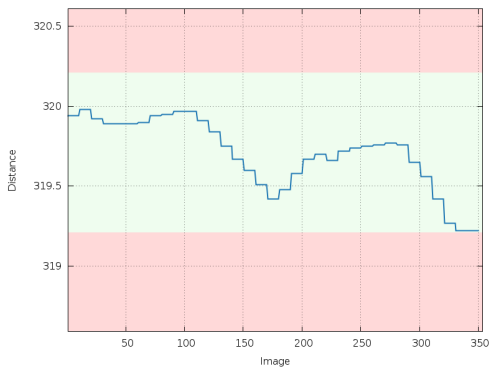


Fig.25 : (sweep 3a) refined crystal-to-detector distance as a function of image number

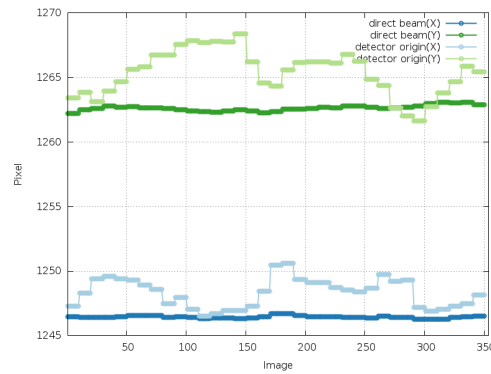


Fig.26 : (sweep 3a) direct beam position and detector origin as a function of image number

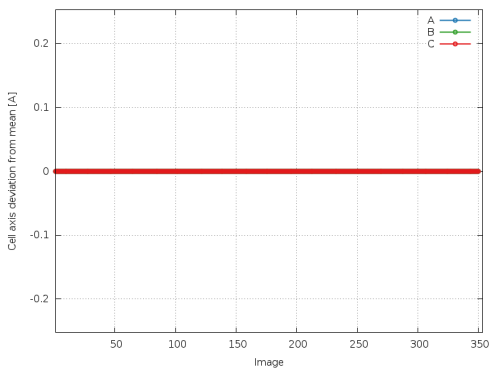


Fig.27 : (sweep 3a) deviation of refined cell axes relative to their mean (as a function of image number)

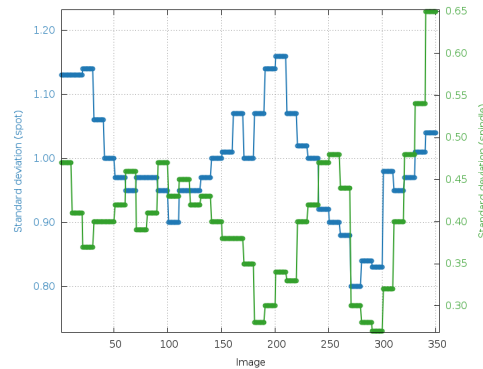


Fig.28 : (sweep 3a) standard deviation (spot position and spindle) as a function of image number

References

- autoPROC Vonrhein, C., Flensburg, C., Keller, P., Sharff, A., Smart, O., Paciorek, W., Womack, T. and Bricogne, G. (2011). Data processing and analysis with the autoPROC toolbox. *Acta Cryst.* D67, 293-302.
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- POINTLESS Evans, P.R. (2006). Scaling and assessment of data quality, *Acta Cryst.* D62, 72-82.
- AIMLESS Evans, P.R. and 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. and 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., and Bricogne, G. (2020). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.