

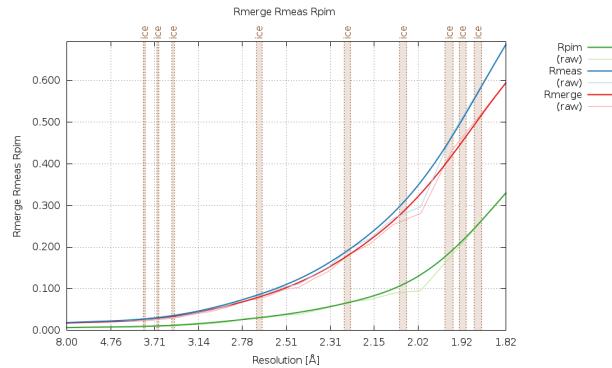
autoPROC	1.1.7 (20190923)
XDS	VERSION Mar 15, 2019 BUILT=20190606
AIMLESS	Version 0.7.4
STARANISO	Version 2.3.13 (7-Sep-2019)
CCP4	Version 7.0.077
Host	server8
User	vonrhein (group = users)
Date	Tue Oct 29 08:36:25 CET 2019
autoPROC	/home/software/xtal/GPhL/20190923 I3_1 #####.cbf (357 images, 53.55°)

## Anisotropic data analysis with STARANISO:

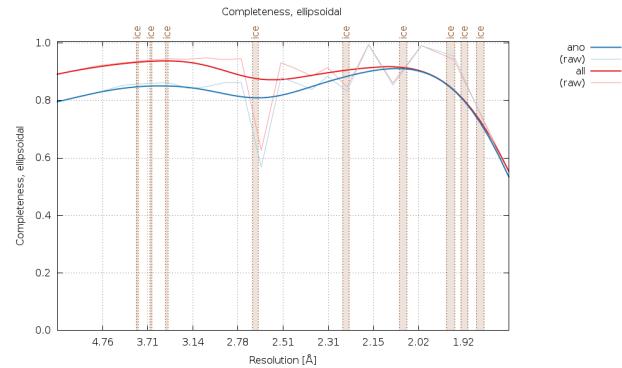
Spacegroup	P6322
Cell parameters	161.201 161.201 139.463 90.0 90.0 120.0
Wavelength [Å]	0.97950
Diffraction limits [Å]	2.330 2.330 1.625
Eigenvector-1	1.000 0.000 0.000
Eigenvector-2	0.000 1.000 0.000
Eigenvector-3	0.000 0.000 1.000
Direction-1	0.894 _a_* - 0.447 _b_*
Direction-2	_b_*
Direction-3	_c_*
Anomalous signal up to	2.9 - 3.3 Å

	Overall	Inner Shell	Outer Shell
Low resolution limit	69.784	69.784	1.898
High resolution limit	1.755	5.674	1.755
Rmerge (all I+ & I-)	0.041	0.018	0.594
Rmeas (all I+ & I-)	0.045	0.019	0.686
Rpim (all I+ & I-)	0.016	0.007	0.330
Total number of observations	408872	18466	11961
Total number unique	61945	3095	3097
Mean(I)/sd(I)	24.8	75.7	1.9
Completeness (spherical)	58.3	89.1	14.1
Completeness (ellipsoidal)	88.5	89.1	55.3
Multiplicity	6.6	6.0	3.9
CC(1/2)	1.000	1.000	0.777
Anomalous completeness (spherical)	54.0	79.5	13.4
Anomalous completeness (ellipsoidal)	82.9	79.5	53.4
Anomalous multiplicity	3.7	3.7	2.1
CC(ano)	0.417	0.782	-0.021
DANO /sd(DANO)	0.903	1.598	0.679

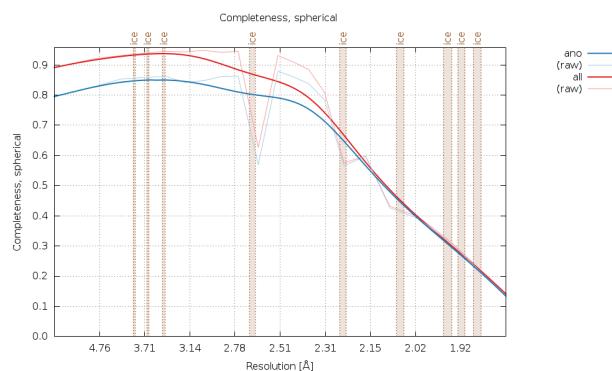
# Final scaling/merging - anisotropic data analysis via STARANISO



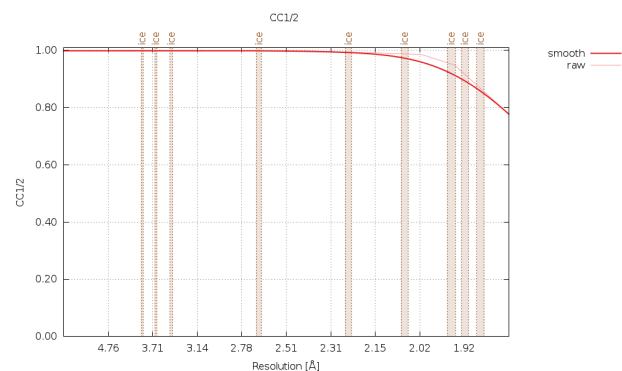
**Fig.1 :** R-values as a function of resolution (observations)



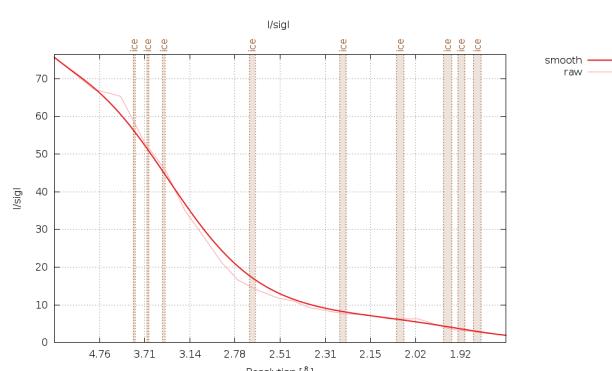
**Fig.2 :** Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.



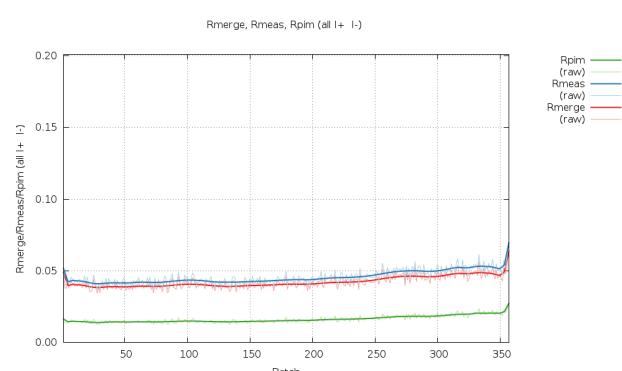
**Fig.3 :** Completeness (spherical) as a function of resolution (observations)



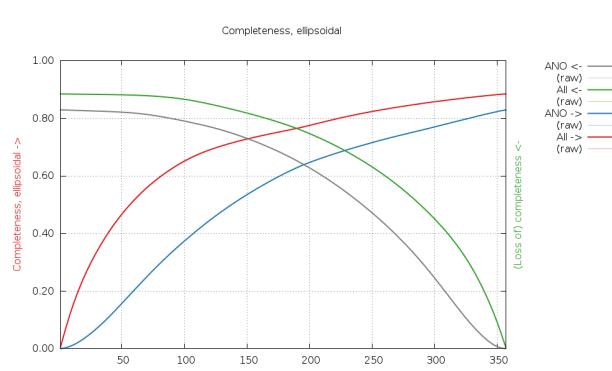
**Fig.4 :** CC1/2 as a function of resolution (observations)



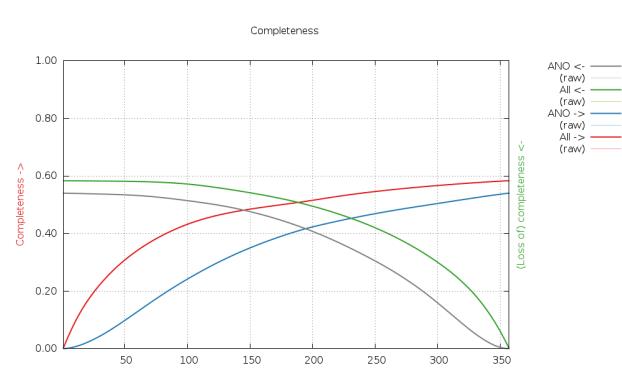
**Fig.5 :** I/sigI as a function of resolution (observations)



**Fig.6 :** R-values as a function of image number (observations)



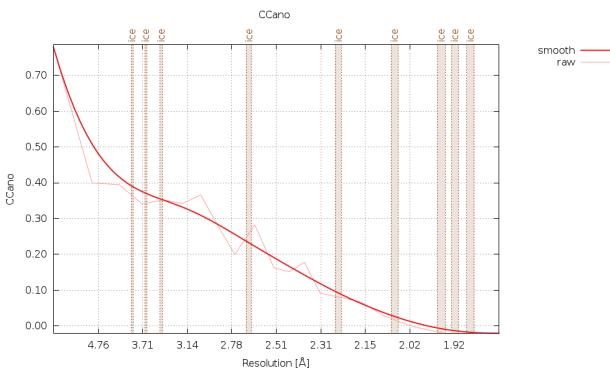
**Fig.7 :** Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.



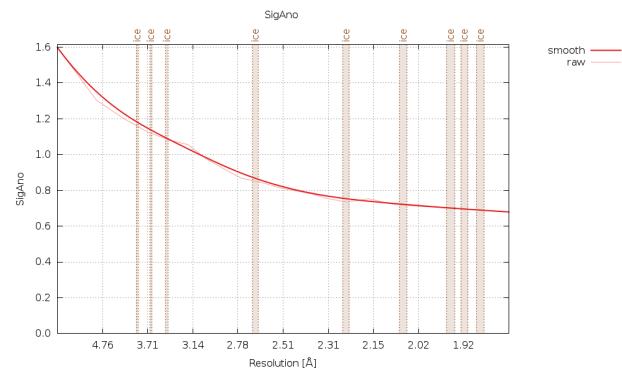
**Fig.8 :** Completeness (spherical) as a function of image number (observations)

## Final scaling/merging - anisotropic data analysis via STARANISO

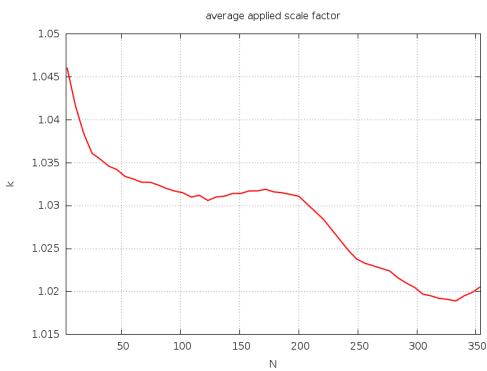
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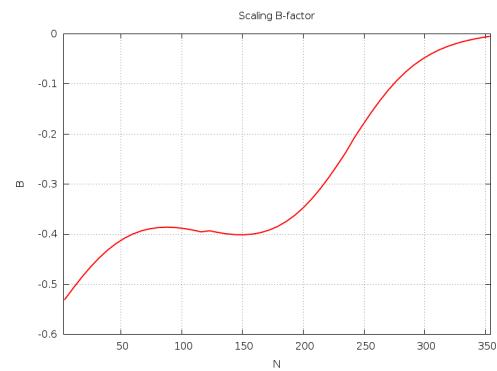
**Fig.9 :** CCano as a function of resolution (observations)



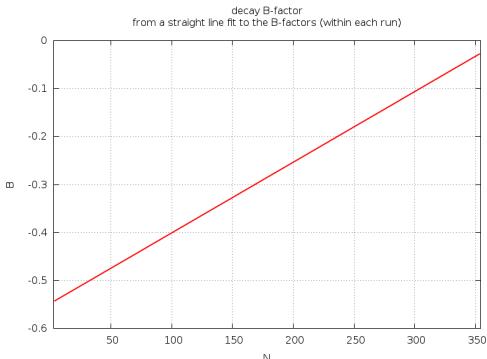
**Fig.10 :** SigAno as a function of resolution (observations)



**Fig.11 :** Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

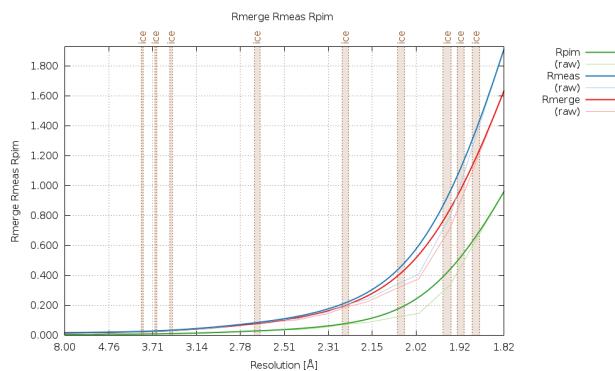


**Fig.12 :** Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

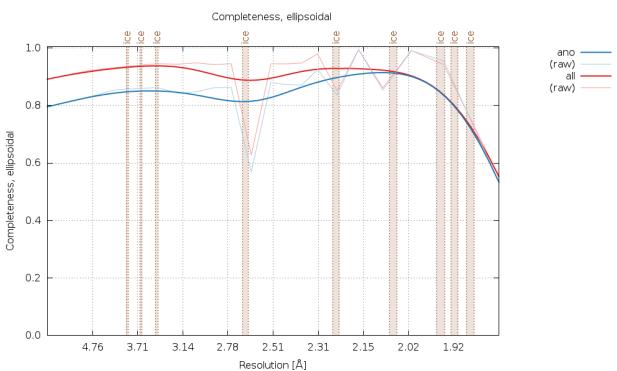


**Fig.13 :** Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

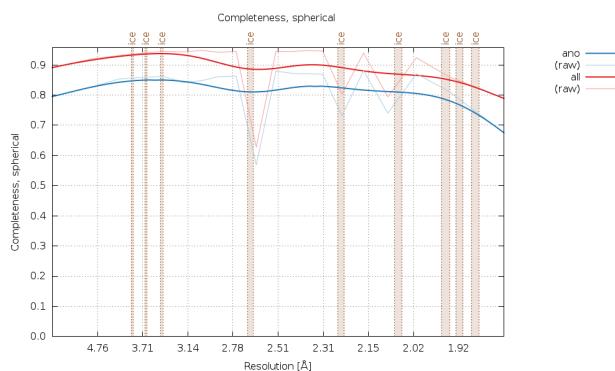
## Final scaling/merging - anisotropic data analysis via STARANISO (all measurements - for comparison only)



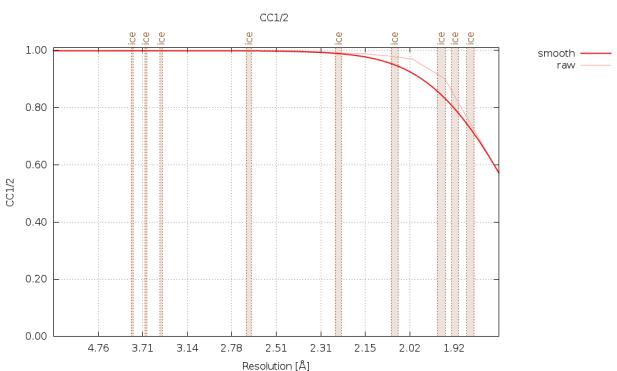
**Fig.14 :** R-values as a function of resolution (measurements)



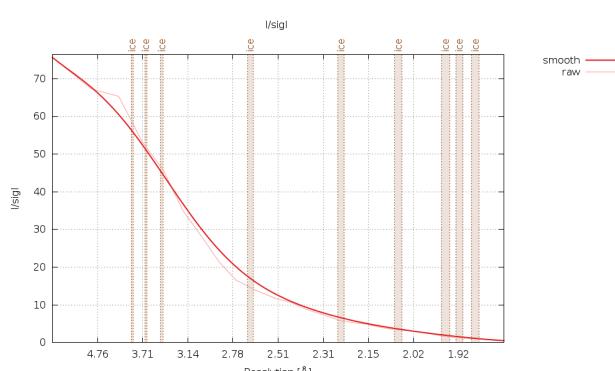
**Fig.15 :** Completeness (ellipsoidal) as a function of resolution (measurements)



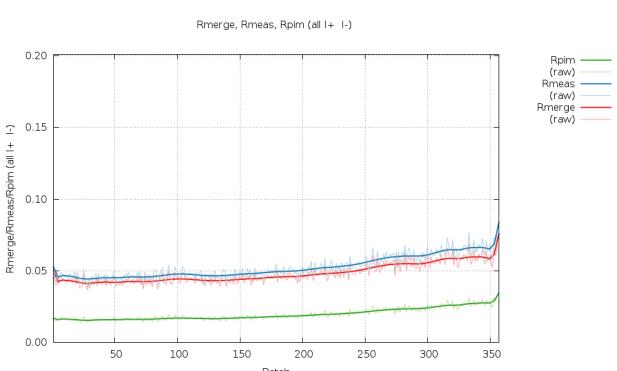
**Fig.16 :** Completeness (spherical) as a function of resolution (measurements)



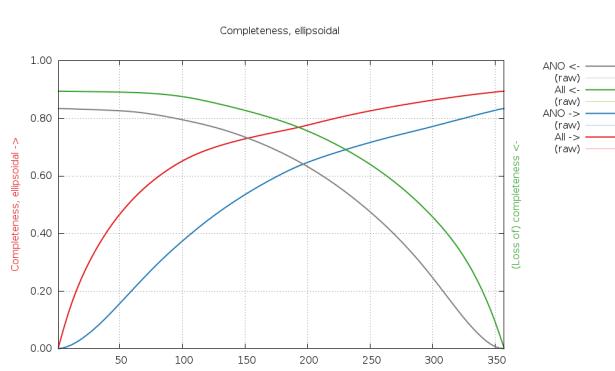
**Fig.17 :** CC1/2 as a function of resolution (measurements)



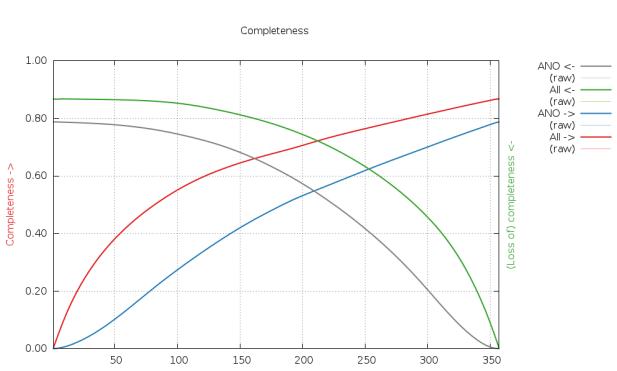
**Fig.18 :** I/sigI as a function of resolution (measurements)



**Fig.19 :** R-values as a function of image number (measurements)

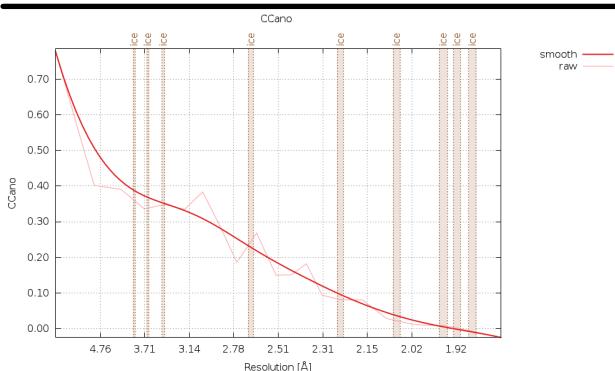


**Fig.20 :** Completeness (ellipsoidal) as a function of image number (measurements)

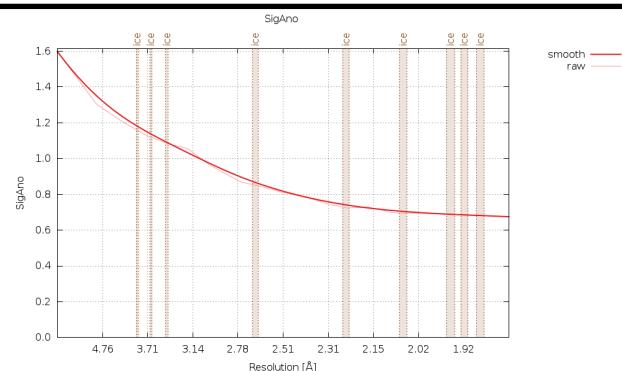


**Fig.21 :** Completeness (spherical) as a function of image number (measurements)

## Final scaling/merging - anisotropic data analysis via STARANISO (all measurements - for comparison only)

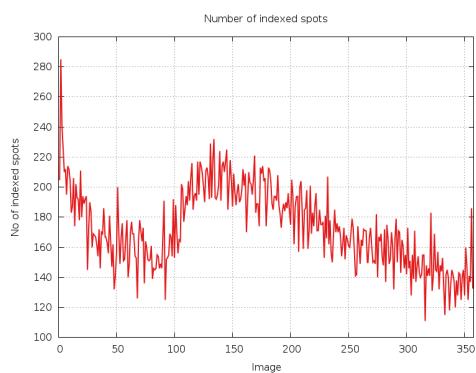


**Fig.22 :** CCano as a function of resolution (measurements)

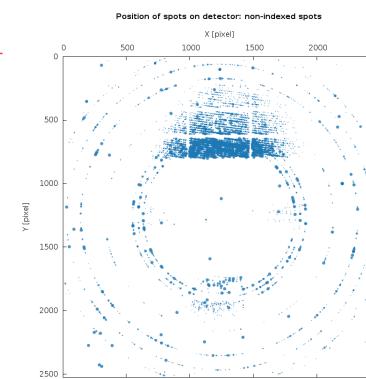


**Fig.23 :** SigAno as a function of resolution (measurements)

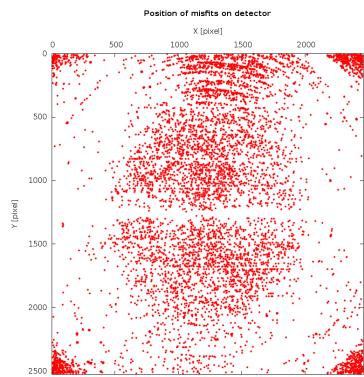
## Data processing



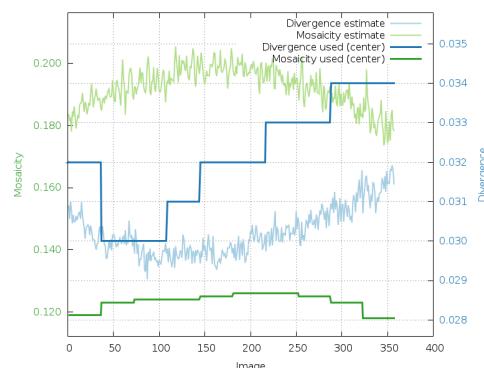
**Fig.24 :** number of spots for each indexing solution as a function of image number



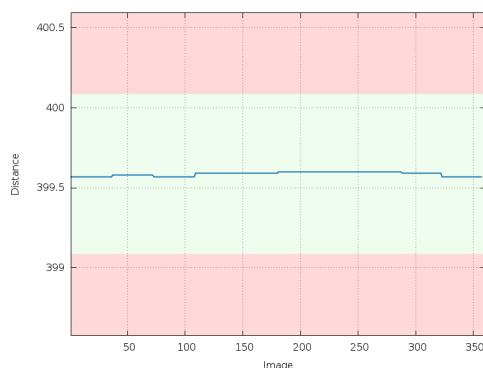
**Fig.25 :** unindexed spots as a function of detector position



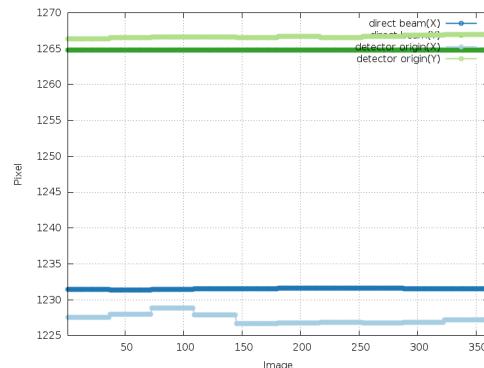
**Fig.26 :** reflections classified as misfits (as a function of detector position)



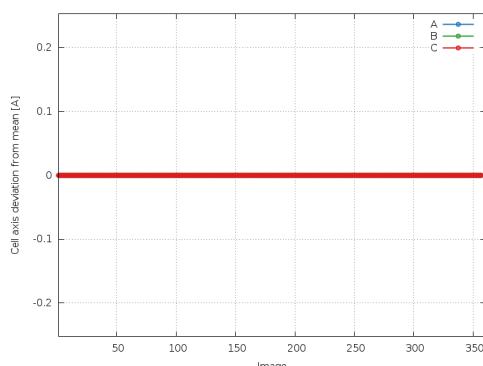
**Fig.27 :** divergence and mosaicity (estimated and used) as a function of image number



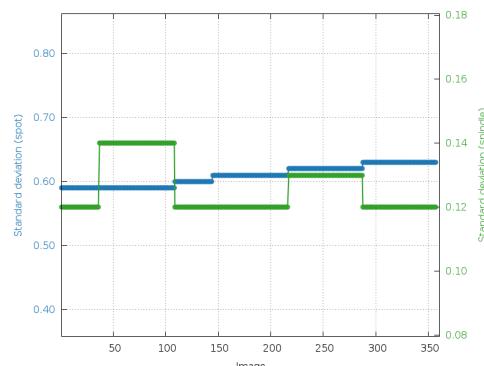
**Fig.28 :** refined crystal-to-detector distance as a function of image number



**Fig.29 :** direct beam position and detector origin as a function of image number



**Fig.30 :** deviation of refined cell axes relative to their mean (as a function of image number)



**Fig.31 :** standard deviation (spot position and spindle) as a function of image number

## References

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- 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.
- 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. 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. (2019). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.