

```

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 Mon Apr 20 10:01:13 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
m4G4eg m4G4eg_#####.cbf (54 images, 27°)
m4G4eg-2 m4G4eg-2_#####.cbf (237 images, 118.5°)
m4G4eg-3 m4G4eg-3_#####.cbf (175 images, 87.5°)
m4G4eg-4 m4G4eg-4_#####.cbf (107 images, 53.5°)
m4G4eg-5 m4G4eg-5_#####.cbf (66 images, 33°)
    
```

### Isotropic data analysis:

```

Spacegroup P3121
Cell parameters 168.5282 168.5282 51.9549
                90.0 90.0 120.0
Wavelength [A] 0.97918
    
```

	Overall	Inner Shell	Outer Shell
Low resolution limit	48.946	48.946	2.173
High resolution limit	2.136	5.796	2.136
Rmerge (all I+ & I-)	0.107	0.062	0.937
Rmeas (all I+ & I-)	0.111	0.064	1.003
Rpim (all I+ & I-)	0.027	0.016	0.354
Total number of observations	708930	41377	18327
Total number unique	47069	2462	2348
Mean(I)/sd(I)	20.1	49.9	2.4
Completeness	100.0	100.0	100.0
Multiplicity	15.1	16.8	7.8
CC(1/2)	0.999	0.999	0.774
Anomalous completeness	99.9	100.0	99.6
Anomalous multiplicity	7.7	9.0	4.0
CC(ano)	-0.148	-0.177	-0.001
DANO /sd(DANO)	0.792	1.084	0.728

# Final scaling/merging - isotropic data analysis

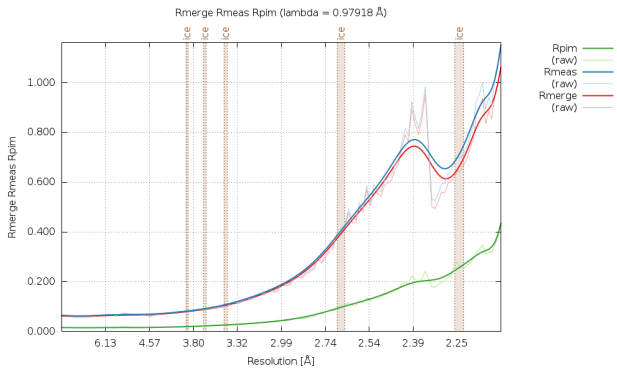


Fig.1 : R-values as a function of resolution

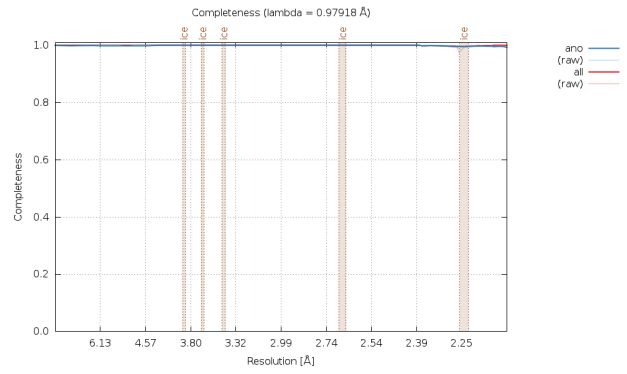


Fig.2 : Completeness as a function of resolution

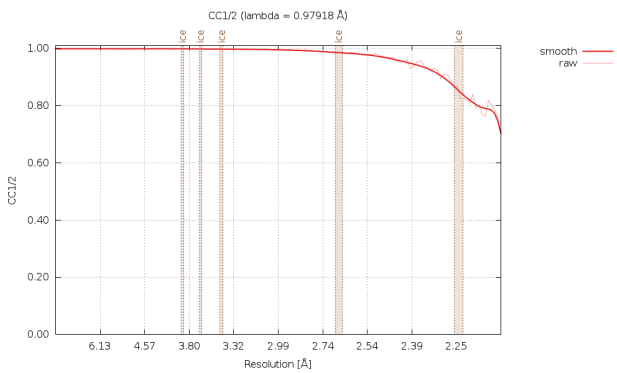


Fig.3 : CC1/2 as a function of resolution

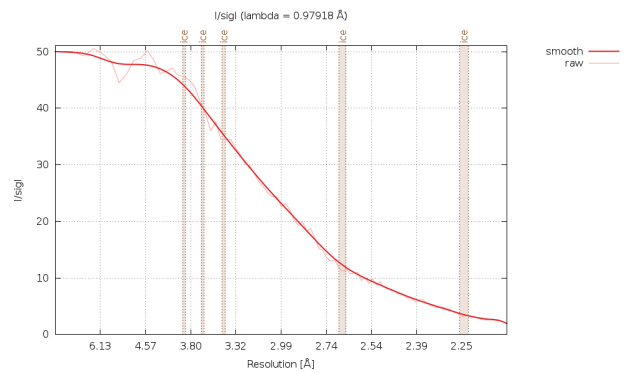


Fig.4 : I/sigI as a function of resolution

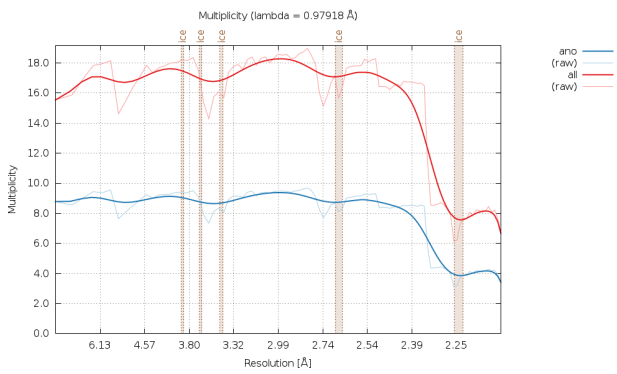


Fig.5 : Multiplicity as a function of resolution

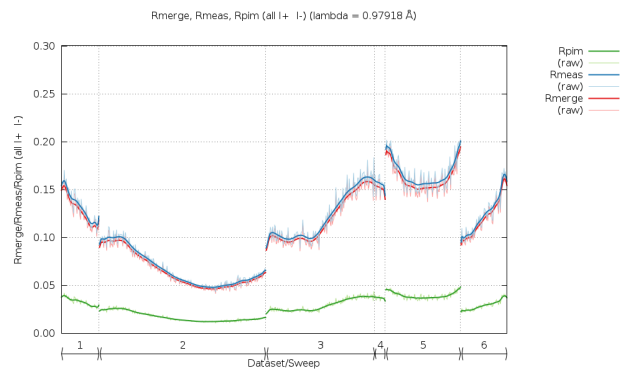


Fig.6 : R-values as a function of image number

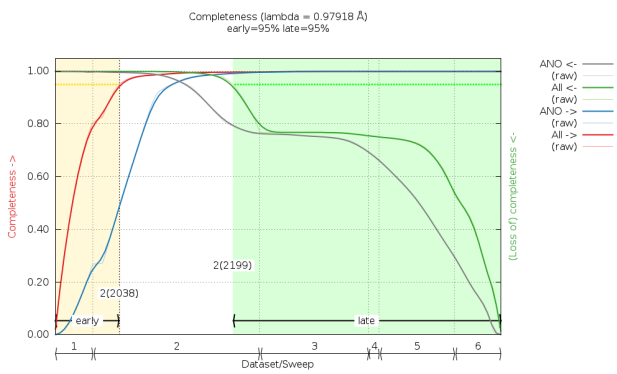


Fig.7 : Completeness as a function of image number

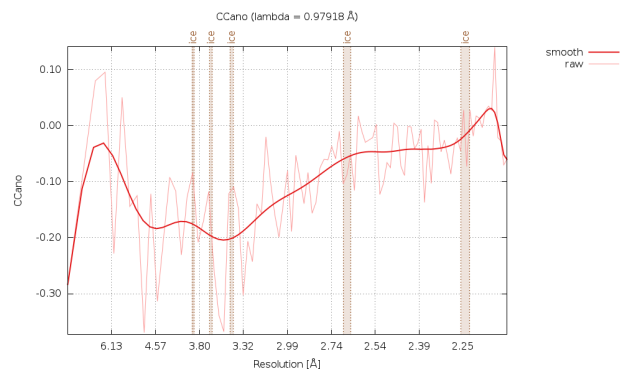


Fig.8 : CCano as a function of resolution

# Final scaling/merging - isotropic data analysis

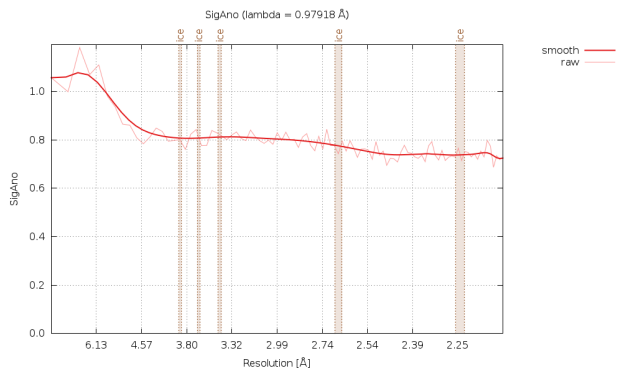


Fig.9 : SigAno as a function of resolution

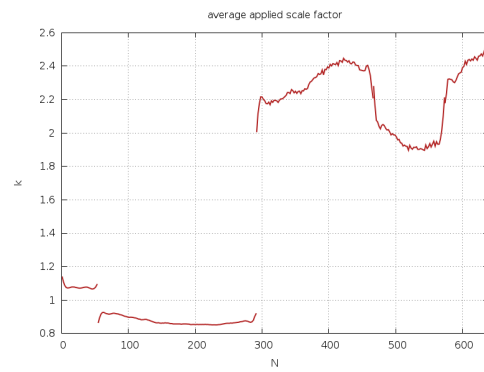


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

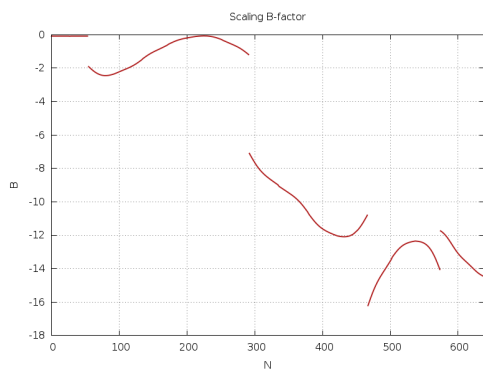


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

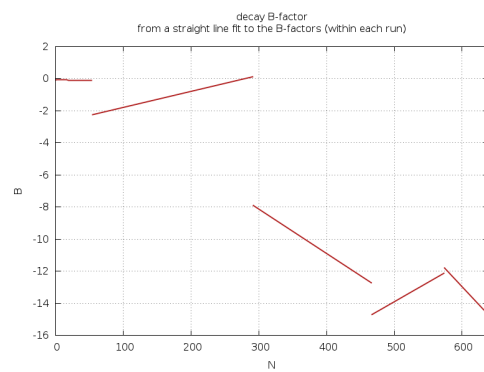
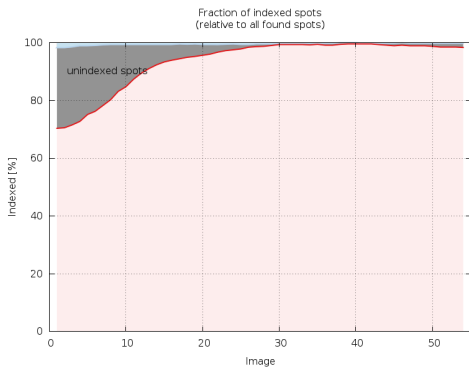
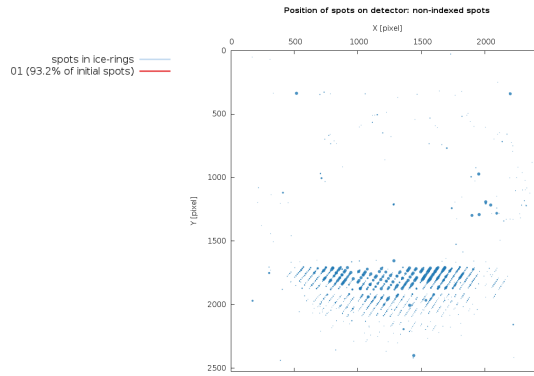


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

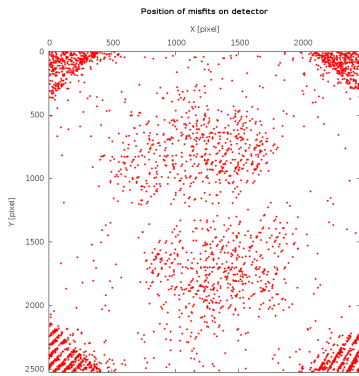
# Data processing sweep m4G4eg



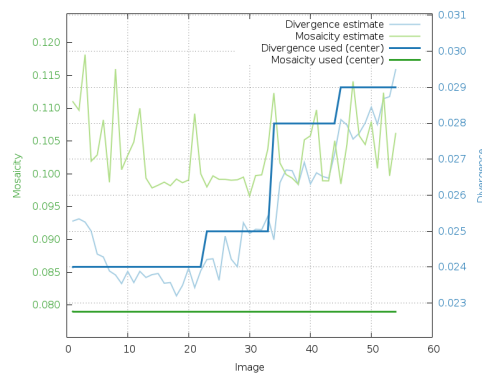
**Fig.13** : (sweep m4G4eg) number of spots for each indexing solution as a function of image number



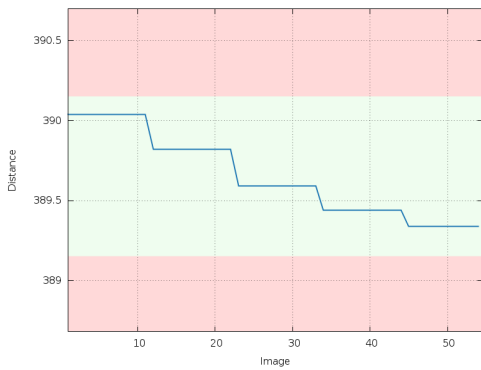
**Fig.14** : (sweep m4G4eg) unindexed spots as a function of detector position



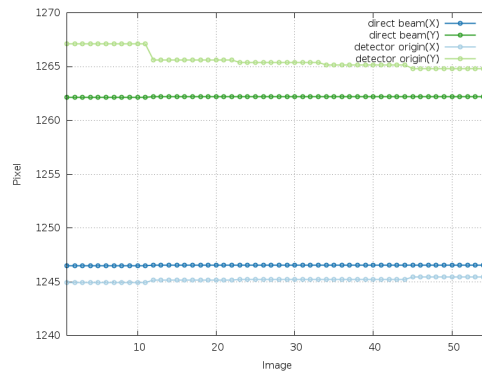
**Fig.15** : (sweep m4G4eg) reflections classified as misfits (as a function of detector position)



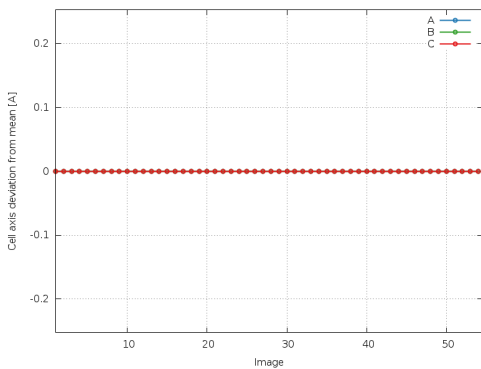
**Fig.16** : (sweep m4G4eg) divergence and mosaicity (estimated and used) as a function of image number



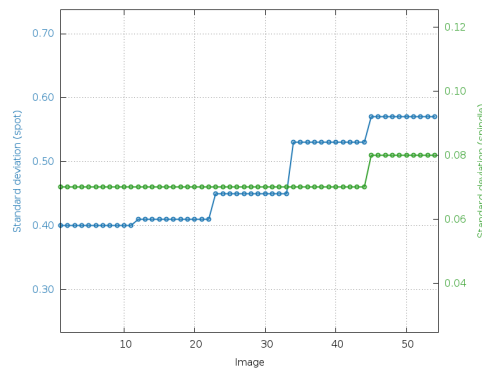
**Fig.17** : (sweep m4G4eg) refined crystal-to-detector distance as a function of image number



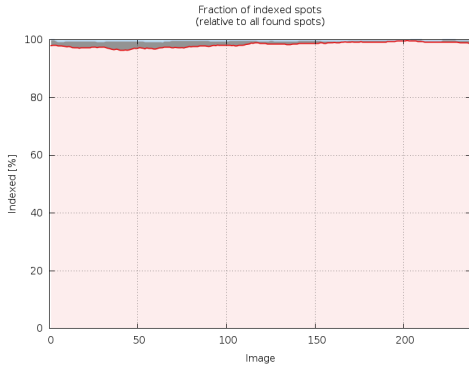
**Fig.18** : (sweep m4G4eg) direct beam position and detector origin as a function of image number



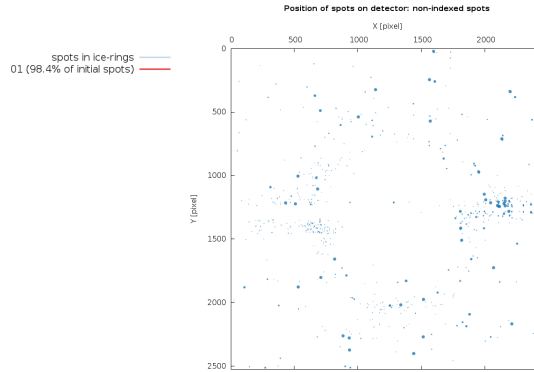
**Fig.19** : (sweep m4G4eg) deviation of refined cell axes relative to their mean (as a function of image number)



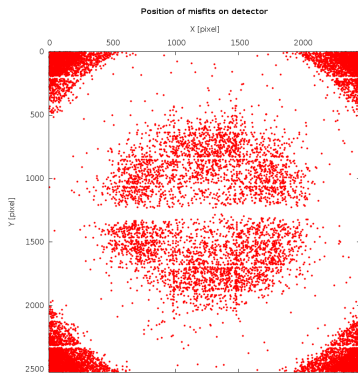
**Fig.20** : (sweep m4G4eg) standard deviation (spot position and spindle) as a function of image number



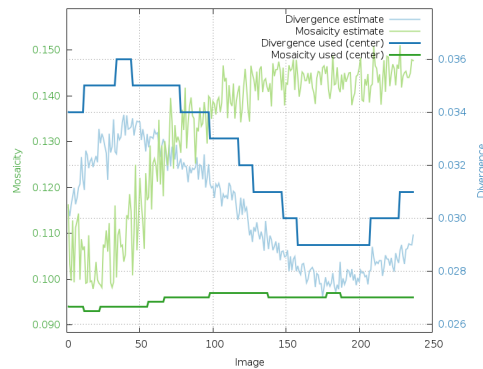
**Fig.21** : (sweep m4G4eg-2) number of spots for each indexing solution as a function of image number



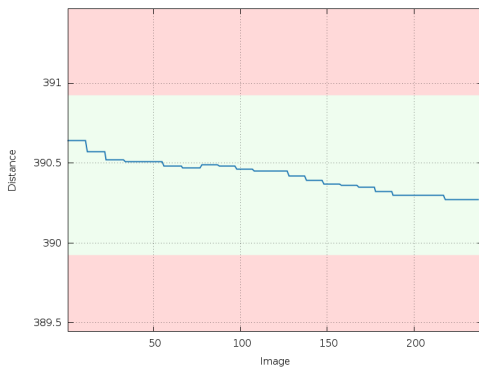
**Fig.22** : (sweep m4G4eg-2) unindexed spots as a function of detector position



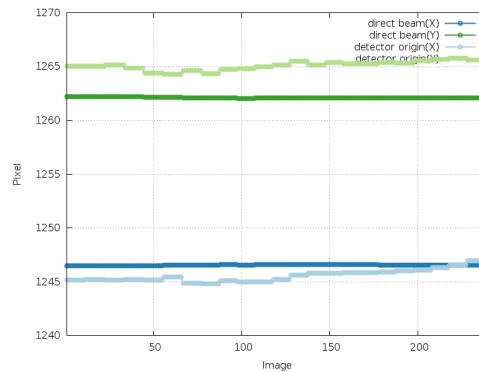
**Fig.23** : (sweep m4G4eg-2) reflections classified as misfits (as a function of detector position)



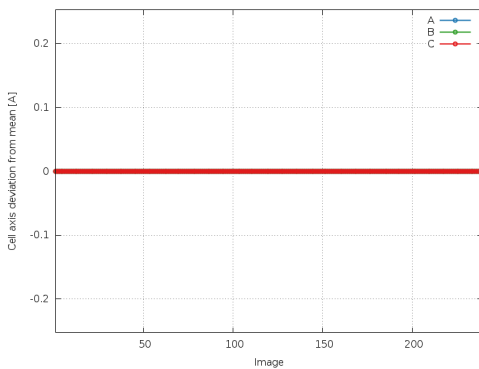
**Fig.24** : (sweep m4G4eg-2) divergence and mosaicity (estimated and used) as a function of image number



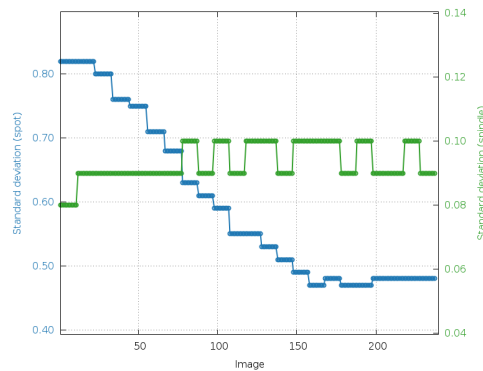
**Fig.25** : (sweep m4G4eg-2) refined crystal-to-detector distance as a function of image number



**Fig.26** : (sweep m4G4eg-2) direct beam position and detector origin as a function of image number



**Fig.27** : (sweep m4G4eg-2) deviation of refined cell axes relative to their mean (as a function of image number)



**Fig.28** : (sweep m4G4eg-2) standard deviation (spot position and spindle) as a function of image number

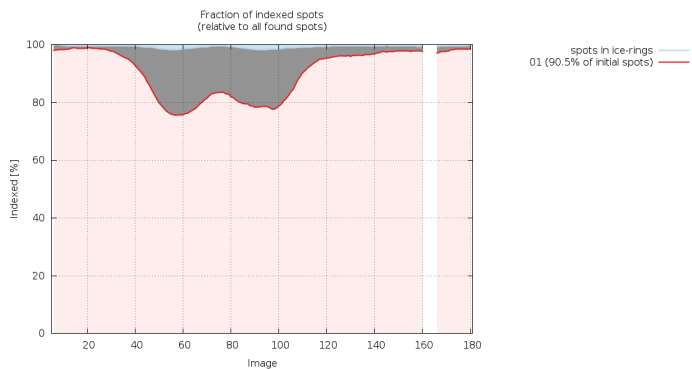


Fig.29 : (sweep m4G4eg-3) number of spots for each indexing solution as a function of image number

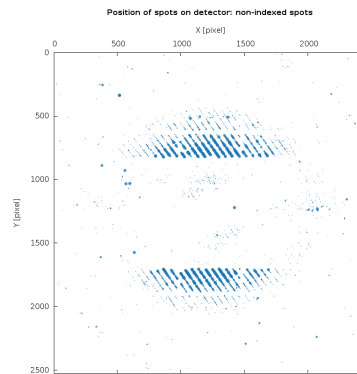


Fig.30 : (sweep m4G4eg-3) unindexed spots as a function of detector position

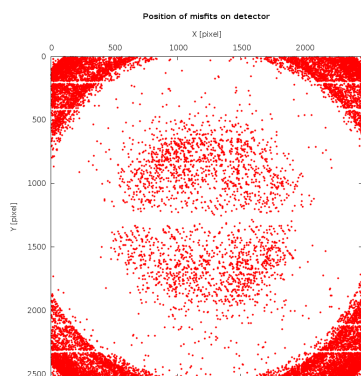


Fig.31 : (sweep m4G4eg-3) reflections classified as misfits (as a function of detector position)

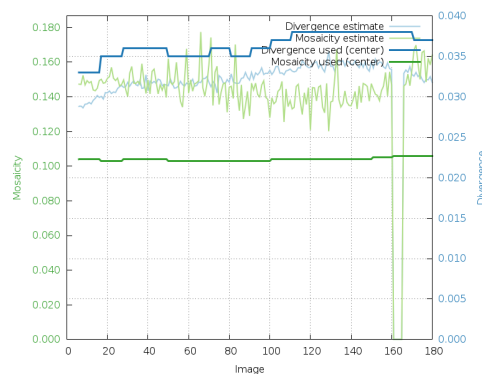


Fig.32 : (sweep m4G4eg-3) divergence and mosaicity (estimated and used) as a function of image number

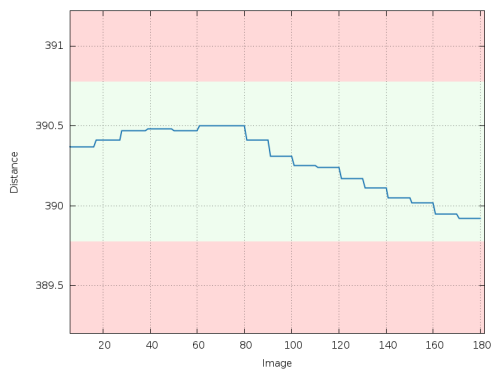


Fig.33 : (sweep m4G4eg-3) refined crystal-to-detector distance as a function of image number

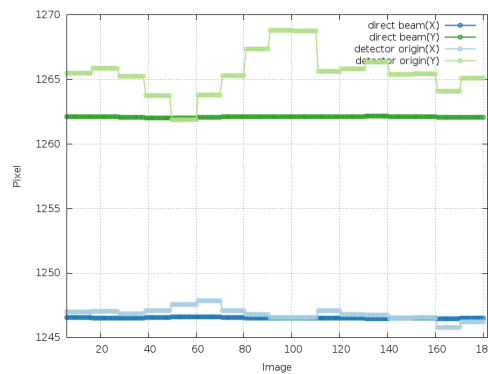


Fig.34 : (sweep m4G4eg-3) direct beam position and detector origin as a function of image number

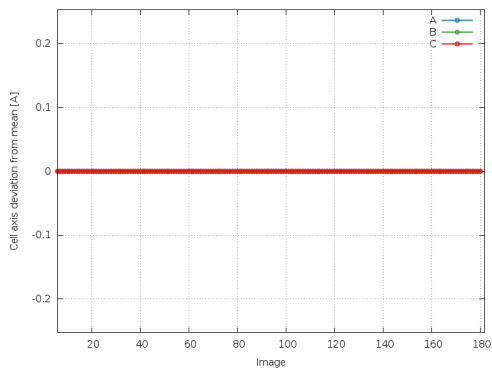


Fig.35 : (sweep m4G4eg-3) deviation of refined cell axes relative to their mean (as a function of image number)

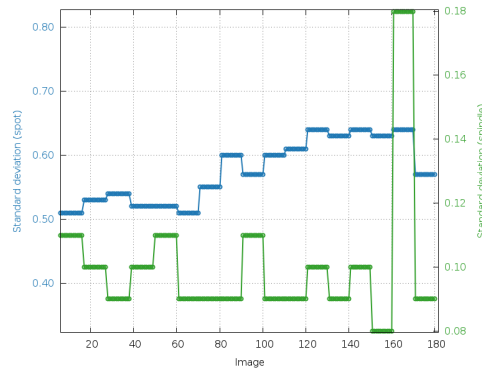
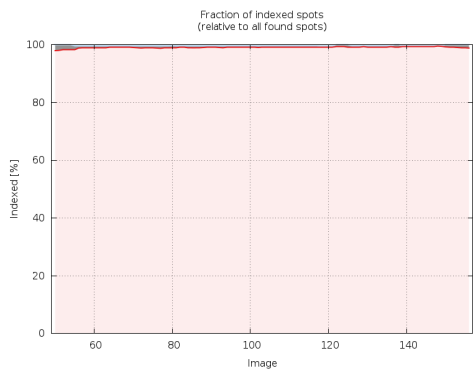
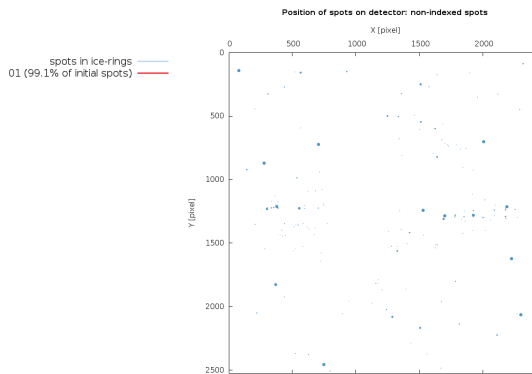


Fig.36 : (sweep m4G4eg-3) standard deviation (spot position and spindle) as a function of image number

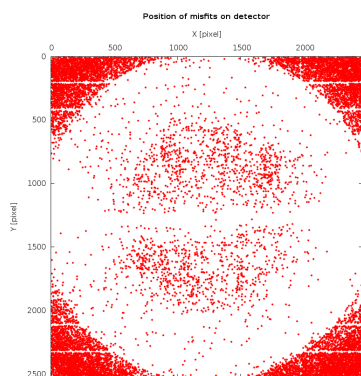
# Data processing sweep m4G4eg-4



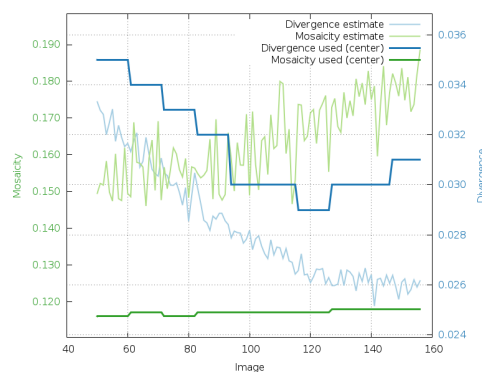
**Fig.37 :** (sweep m4G4eg-4) number of spots for each indexing solution as a function of image number



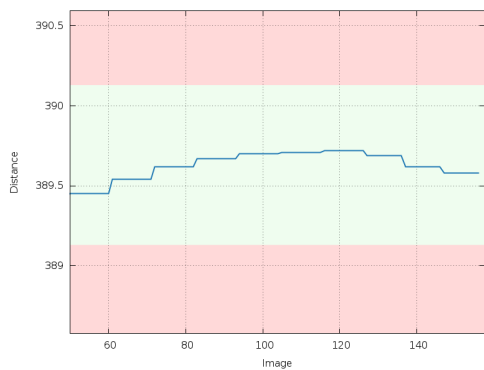
**Fig.38 :** (sweep m4G4eg-4) unindexed spots as a function of detector position



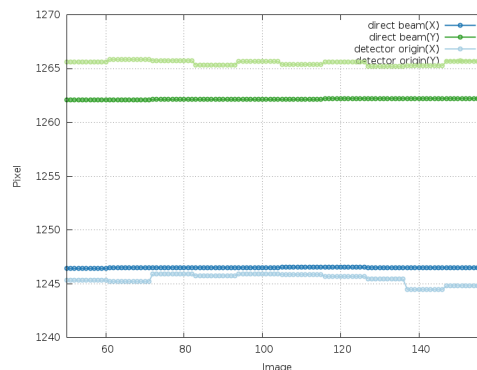
**Fig.39 :** (sweep m4G4eg-4) reflections classified as misfits (as a function of detector position)



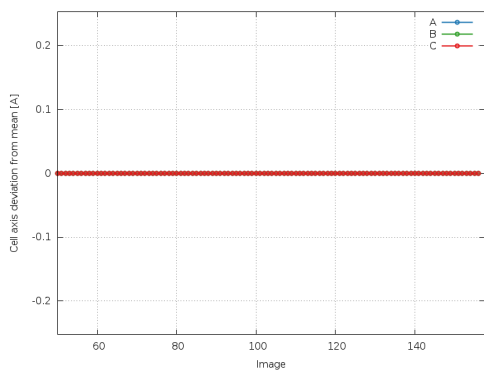
**Fig.40 :** (sweep m4G4eg-4) divergence and mosaicity (estimated and used) as a function of image number



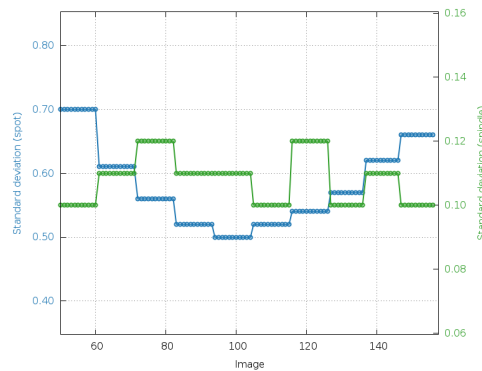
**Fig.41 :** (sweep m4G4eg-4) refined crystal-to-detector distance as a function of image number



**Fig.42 :** (sweep m4G4eg-4) direct beam position and detector origin as a function of image number

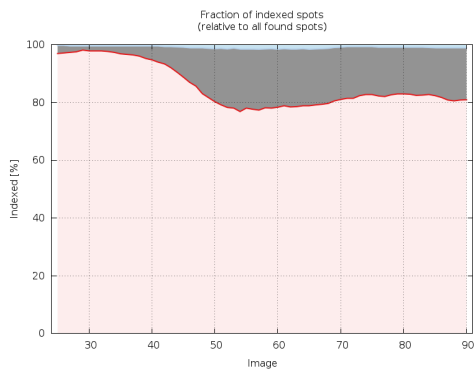


**Fig.43 :** (sweep m4G4eg-4) deviation of refined cell axes relative to their mean (as a function of image number)

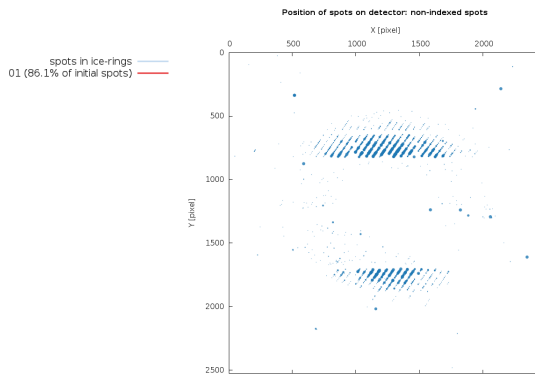


**Fig.44 :** (sweep m4G4eg-4) standard deviation (spot position and spindle) as a function of image number

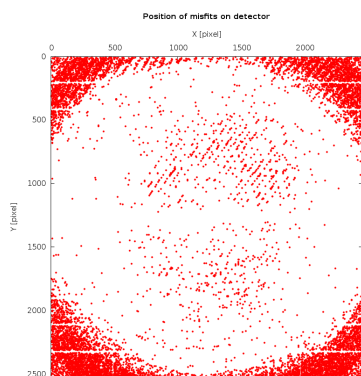
# Data processing sweep m4G4eg-5



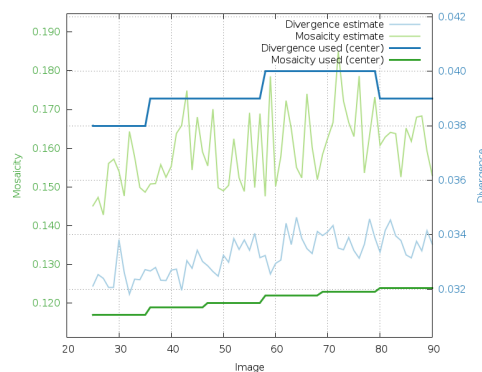
**Fig.45 :** (sweep m4G4eg-5) number of spots for each indexing solution as a function of image number



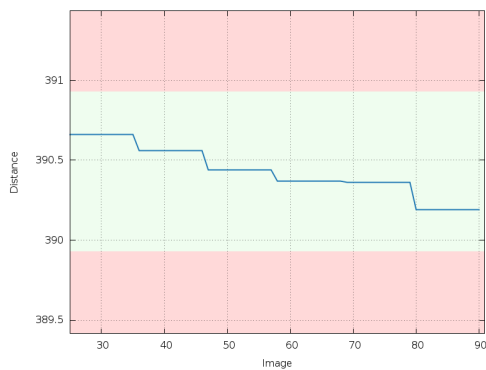
**Fig.46 :** (sweep m4G4eg-5) unindexed spots as a function of detector position



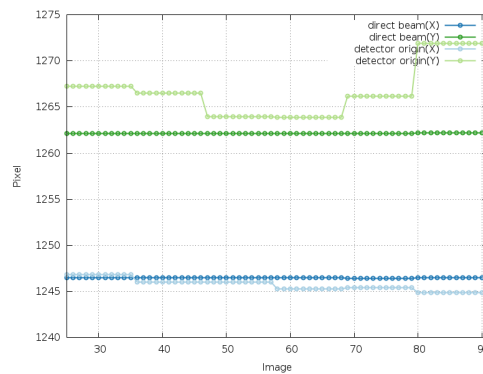
**Fig.47 :** (sweep m4G4eg-5) reflections classified as misfits (as a function of detector position)



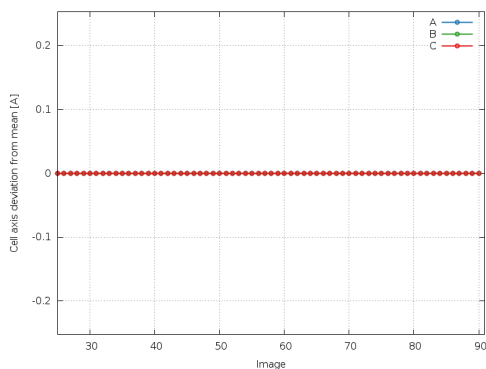
**Fig.48 :** (sweep m4G4eg-5) divergence and mosaicity (estimated and used) as a function of image number



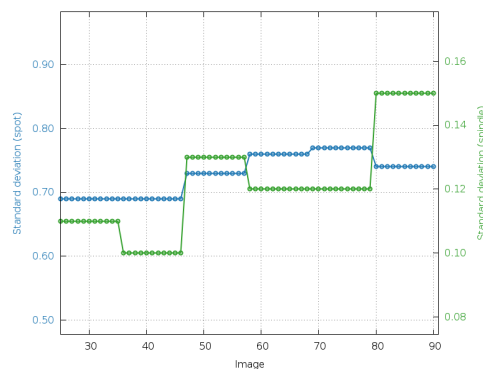
**Fig.49 :** (sweep m4G4eg-5) refined crystal-to-detector distance as a function of image number



**Fig.50 :** (sweep m4G4eg-5) direct beam position and detector origin as a function of image number



**Fig.51 :** (sweep m4G4eg-5) deviation of refined cell axes relative to their mean (as a function of image number)



**Fig.52 :** (sweep m4G4eg-5) 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.
- 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. (2020). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.