

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°)

Isotropic data analysis:

Spacegroup	P6322
Cell parameters	161.201 161.201 139.463 90.0 90.0 120.0
Wavelength [Å]	0.97950
Anomalous signal up to	2.9 - 3.3 Å

	Overall	Inner Shell	Outer Shell
Low resolution limit	69.784	69.784	2.001
High resolution limit	1.967	5.339	1.967
Rmerge (all I+ & I-)	0.042	0.018	0.462
Rmeas (all I+ & I-)	0.045	0.020	0.503
Rpim (all I+ & I-)	0.016	0.007	0.191
Total number of observations	420171	21806	20183
Total number unique	67668	3689	3375
Mean(I)/sd(I)	22.6	73.8	2.4
Completeness	89.2	89.5	90.7
Multiplicity	6.2	5.9	6.0
CC(1/2)	1.000	1.000	0.957
Anomalous completeness	81.9	79.9	84.9
Anomalous multiplicity	3.5	3.6	3.3
CC(ano)	0.421	0.786	-0.021
DANO /sd(DANO)	0.888	1.561	0.694

Final scaling/merging - isotropic data analysis

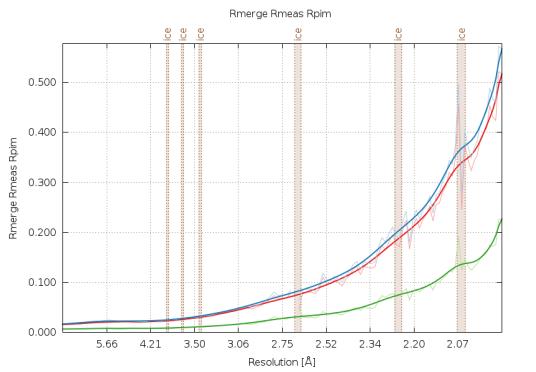


Fig.1 : R-values as a function of resolution

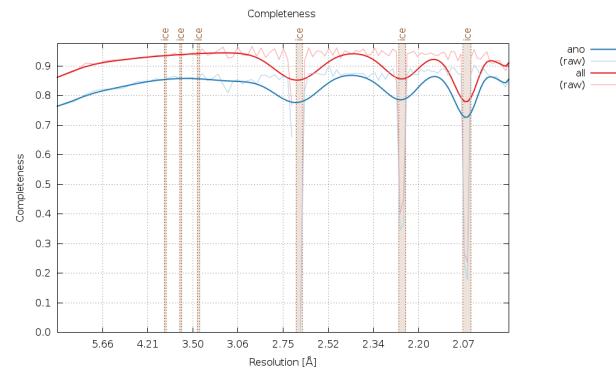


Fig.2 : Completeness as a function of resolution

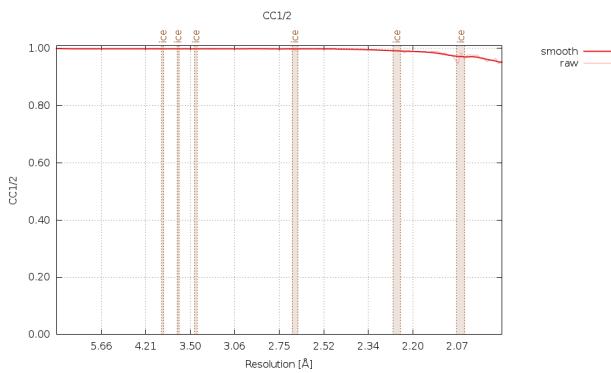


Fig.3 : CC_{1/2} as a function of resolution

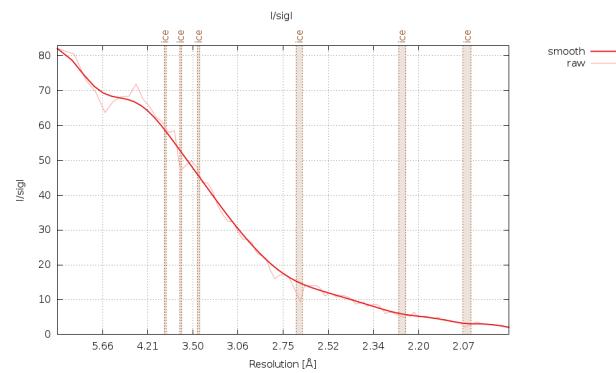


Fig.4 : I/sigI as a function of resolution

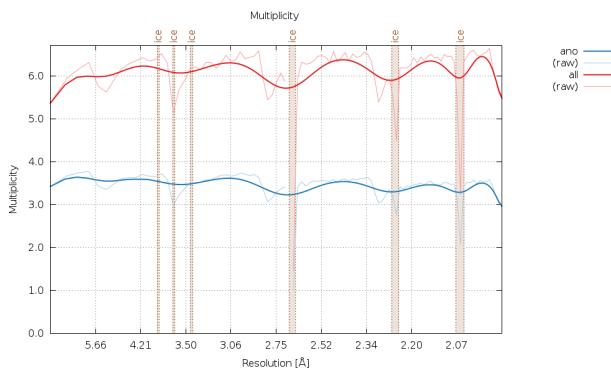


Fig.5 : Multiplicity as a function of resolution

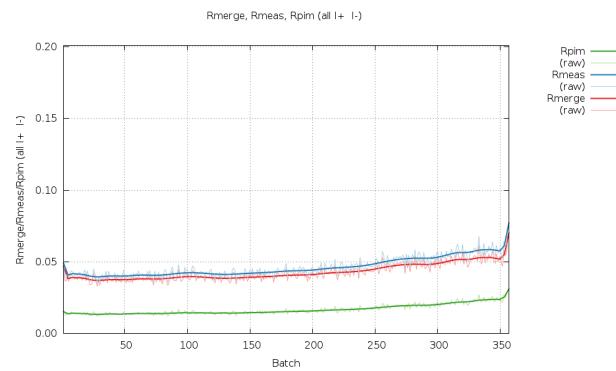


Fig.6 : R-values as a function of image number

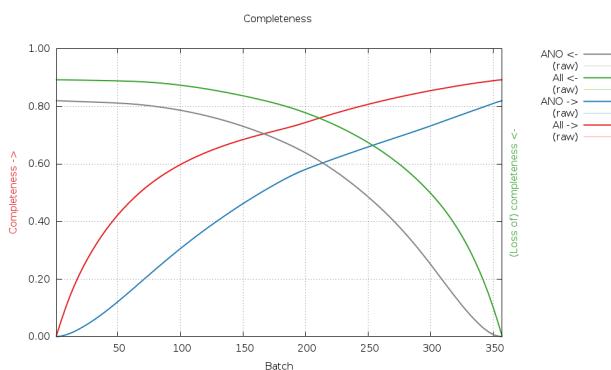


Fig.7 : Completeness as a function of image number

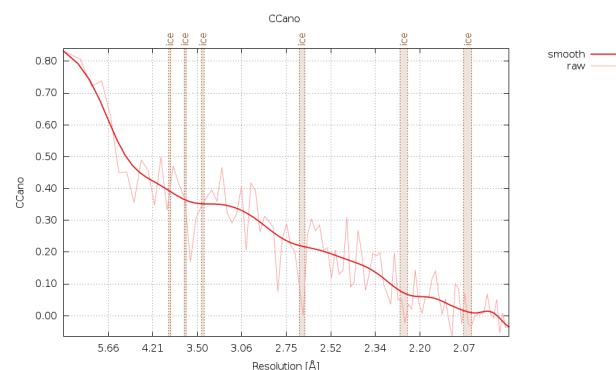


Fig.8 : CC_{ano} as a function of resolution

Final scaling/merging - isotropic data analysis

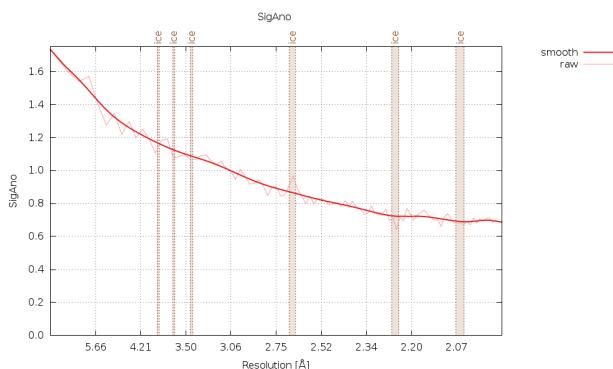


Fig.9 : SigAno as a function of resolution

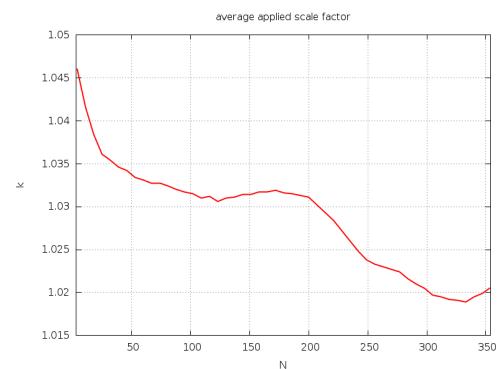


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

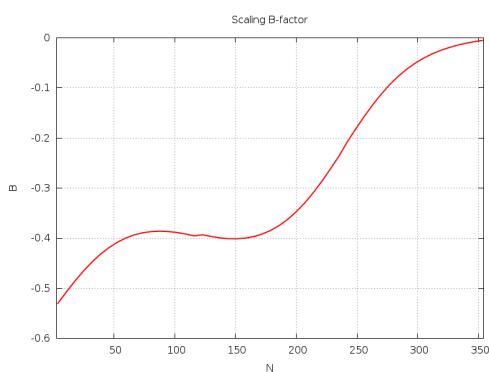


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

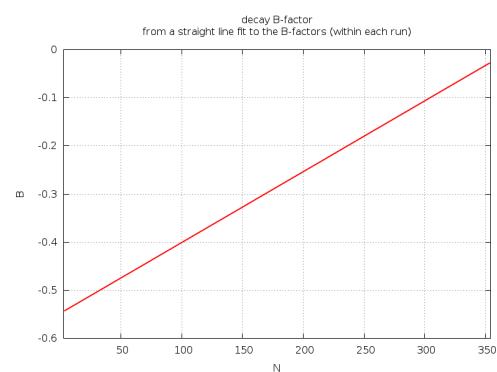


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

Data processing

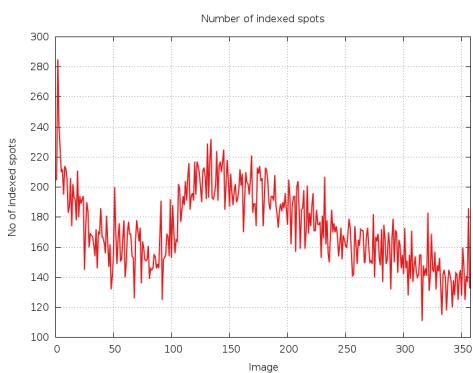


Fig.13 : number of spots for each indexing solution as a function of image number

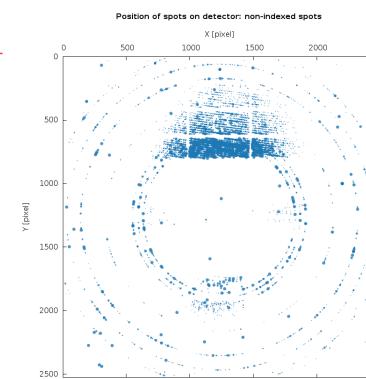


Fig.14 : unindexed spots as a function of detector position

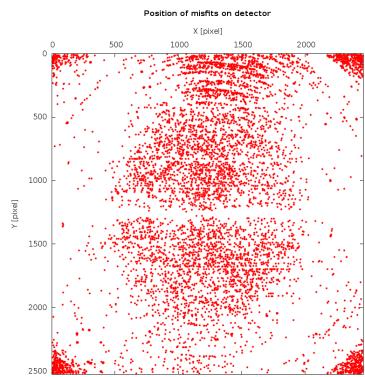


Fig.15 : reflections classified as misfits (as a function of detector position)

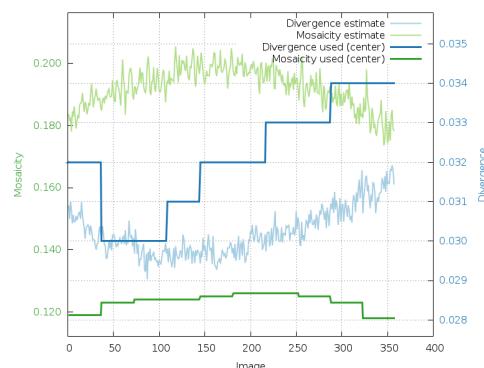


Fig.16 : divergence and mosaicity (estimated and used) as a function of image number

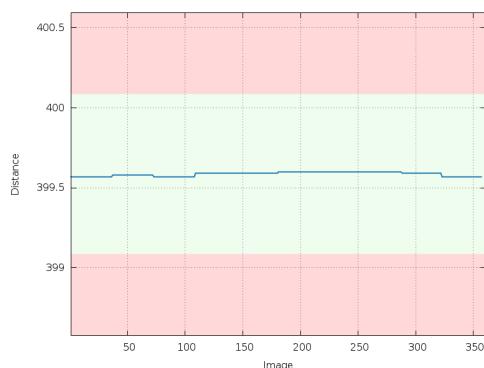


Fig.17 : refined crystal-to-detector distance as a function of image number

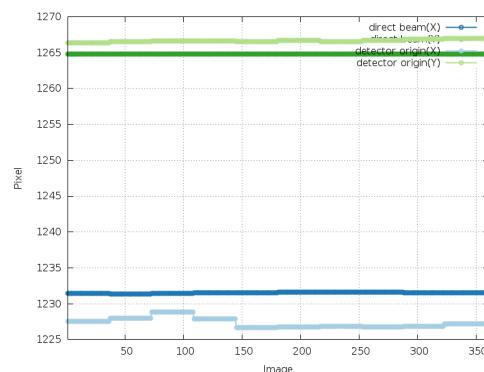


Fig.18 : direct beam position and detector origin as a function of image number

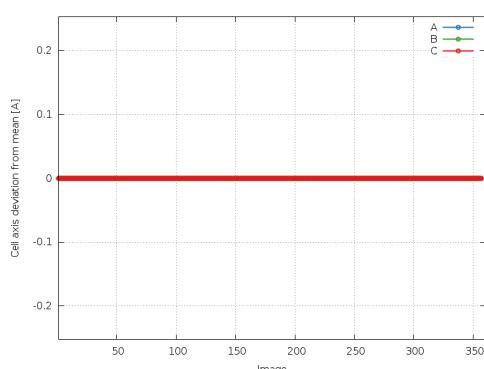


Fig.19 : deviation of refined cell axes relative to their mean (as a function of image number)

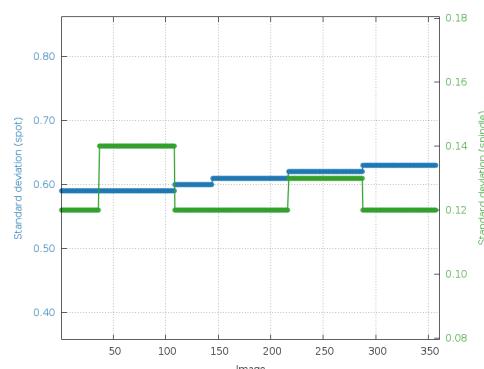


Fig.20 : standard deviation (spot position and spindle) as a function of image number

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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- 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.
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