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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 Fri Apr 24 08:42:24 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
ADRP_Pmin_F11_d1_ ADRP_Pmin_F11_d1_data #####.cbf (720
data images, 360°)
ADRP_Pmin_F11_d1_ ADRP_Pmin_F11_d1_data2 #####.cbf (200
data2 images, 100°)
    
```

Isotropic data analysis:

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Spacegroup C2
Cell parameters 139.5938 29.6609 37.8595
                90.0000 103.5076 90.0000
Wavelength [A] 0.97918
    
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	Overall	Inner Shell	Outer Shell
Low resolution limit	36.083	36.083	1.145
High resolution limit	1.125	3.054	1.125
Rmerge (all I+ & I-)	0.122	0.056	0.852
Rmeas (all I+ & I-)	0.133	0.060	1.096
Rpim (all I+ & I-)	0.052	0.021	0.683
Total number of observations	274299	24056	4995
Total number unique	53290	2974	2549
Mean(I)/sd(I)	10.8	33.9	1.0
Completeness	92.5	98.4	87.5
Multiplicity	5.1	8.1	2.0
CC(1/2)	0.994	0.998	0.324
Anomalous completeness	67.2	99.3	36.3
Anomalous multiplicity	3.3	4.3	1.4
CC(ano)	-0.102	-0.171	NA
DANO /sd(DANO)	0.725	0.687	0.657

Final scaling/merging - isotropic data analysis

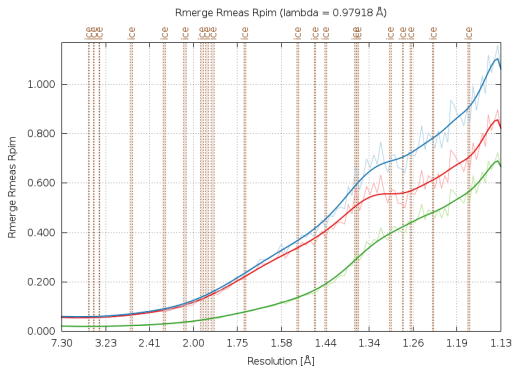


Fig.1 : R-values as a function of resolution

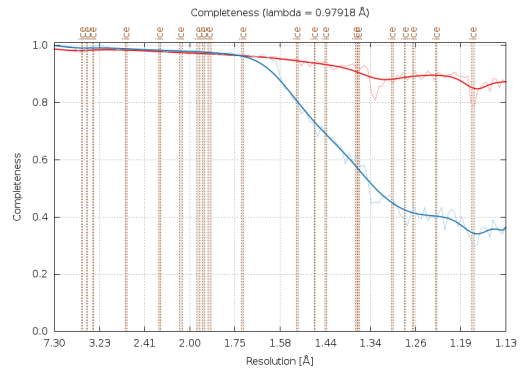


Fig.2 : Completeness as a function of resolution

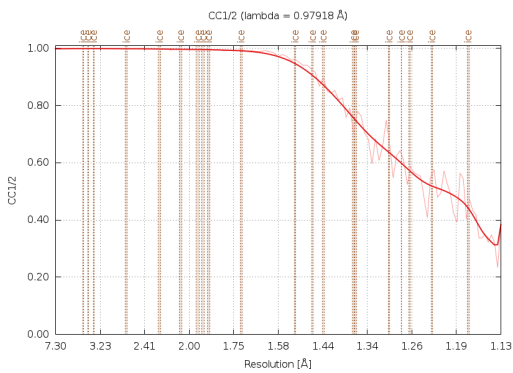


Fig.3 : CC1/2 as a function of resolution

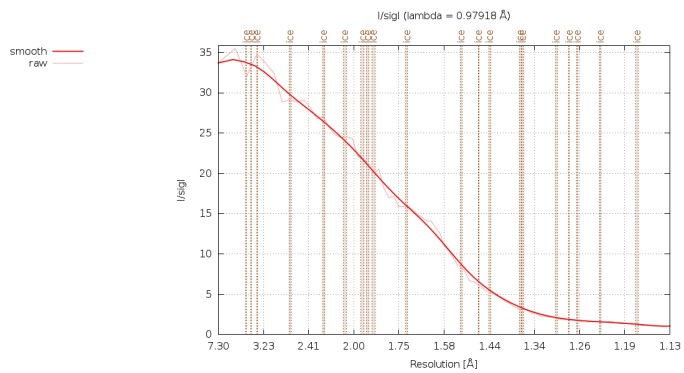


Fig.4 : I/sigI as a function of resolution

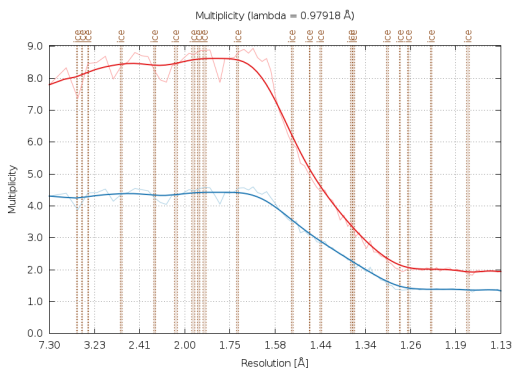


Fig.5 : Multiplicity as a function of resolution

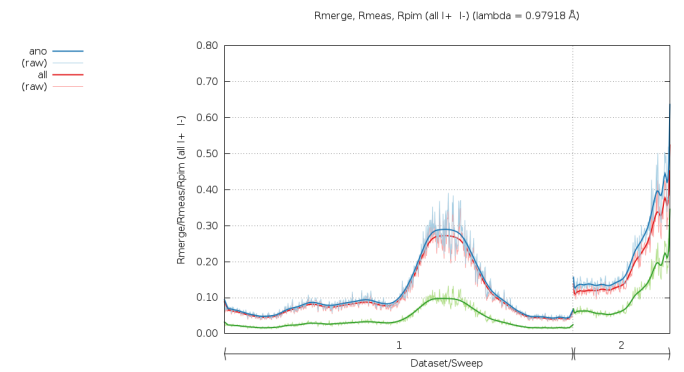


Fig.6 : R-values as a function of image number

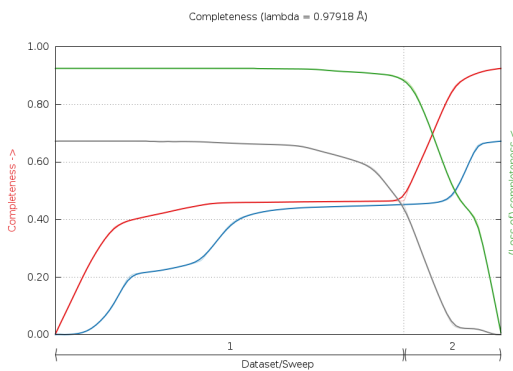


Fig.7 : Completeness as a function of image number

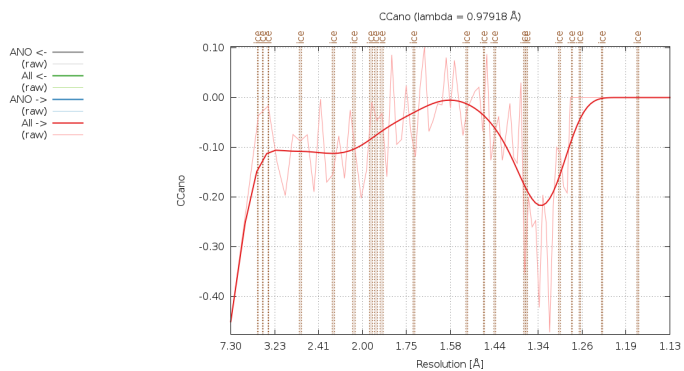


Fig.8 : CCano as a function of resolution

Final scaling/merging - isotropic data analysis

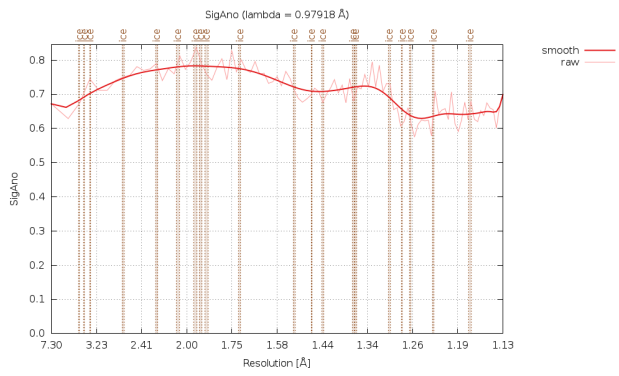


Fig.9 : SigAno as a function of resolution

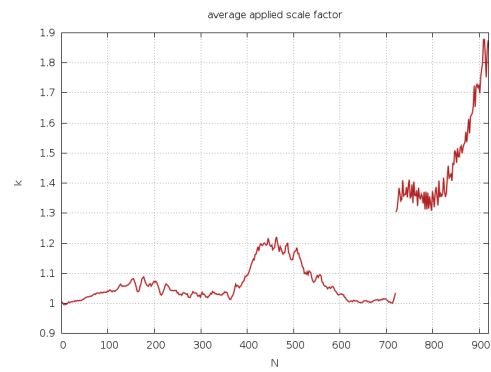


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

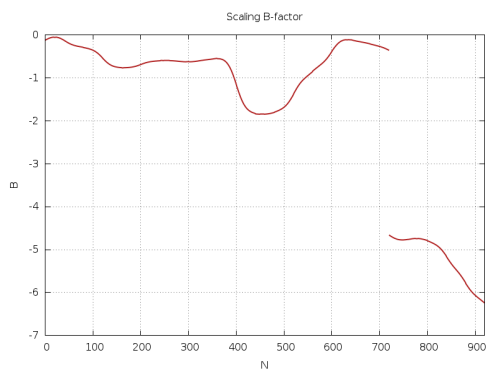


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

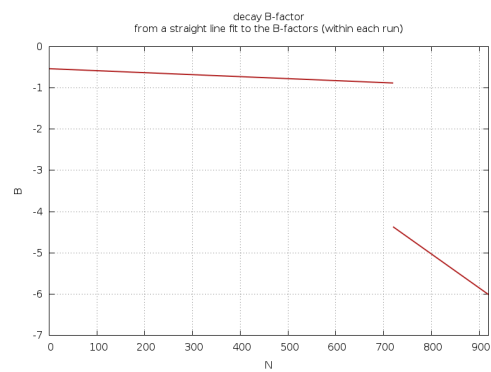


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

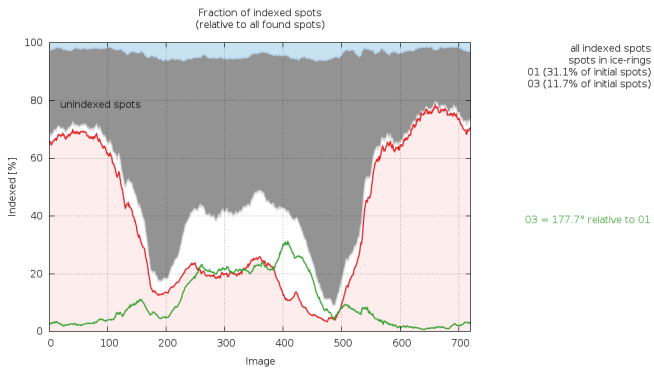


Fig.13 : (sweep ADRP_Pmin_F11_d1_data) number of spots for each indexing solution as a function of image number

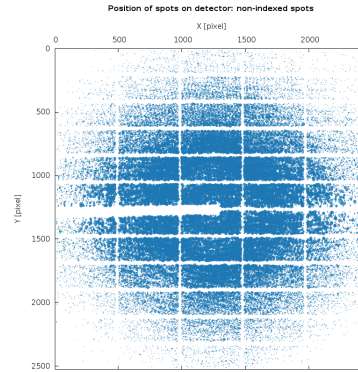


Fig.14 : (sweep ADRP_Pmin_F11_d1_data) unindexed spots as a function of detector position

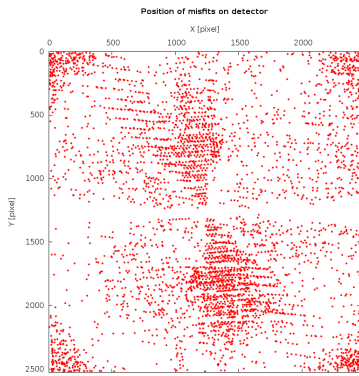


Fig.15 : (sweep ADRP_Pmin_F11_d1_data) reflections classified as misfits (as a function of detector position)

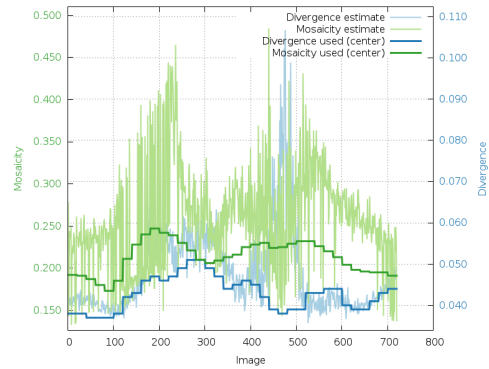
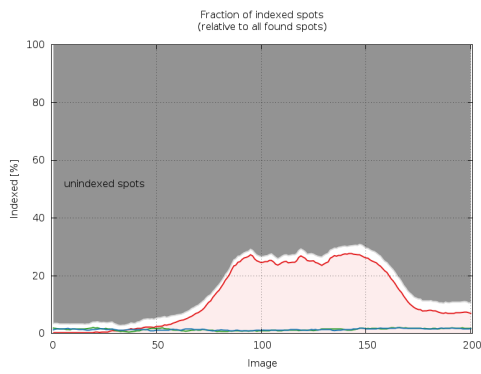


Fig.16 : (sweep ADRP_Pmin_F11_d1_data) divergence and mosaicity (estimated and used) as a function of image number



all indexed spots
 O1 (12.6% of initial spots)
 O2 (1.5% of initial spots)
 O3 (1.5% of initial spots)

O2 = 12.2° relative to O1
 O3 = 11.3° relative to O1

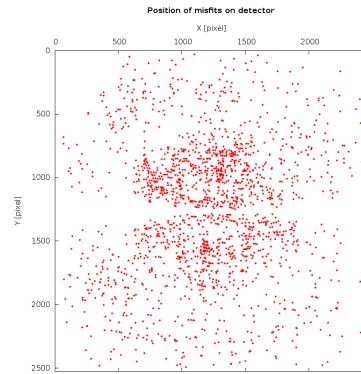


Fig.17 : (sweep ADRP_Pmin_F11_d1_data2) number of spots for each indexing solution as a function of image number

Fig.18 : (sweep ADRP_Pmin_F11_d1_data2) reflections classified as misfits (as a function of detector position)

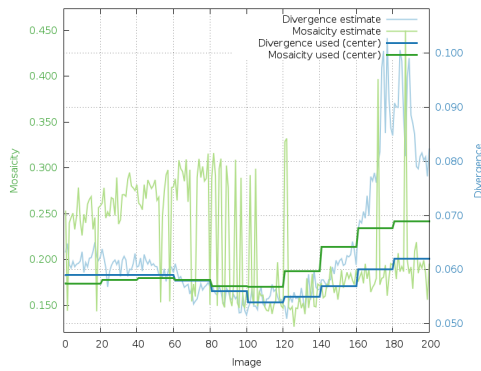


Fig.19 : (sweep ADRP_Pmin_F11_d1_data2) divergence and mosaicity (estimated and used) as a function of image number

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.