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autoPROC 1.1.7 (20200319)
XDS VERSION Jan 31, 2020 BUILT=20200131
AIMLESS Version 0.7.4
STARANISO Version 2.3.28 (1-Mar-2020)
CCP4 Version 7.0.078
Host server8
User vonrhein (group = users)
Date Thu Mar 19 13:30:31 CET 2020
autoPROC /home/software/xtal/GPhL/20200319
P1P7_G4_X1_#####.cbf (1199 images, 179.85°)
    
```

Isotropic data analysis:

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Spacegroup P212121
Cell parameters 80.907 88.869 128.704
                90.0 90.0 90.0
Wavelength [A] 0.97926
    
```

	Overall	Inner Shell	Outer Shell
Low resolution limit	73.130	73.130	1.705
High resolution limit	1.676	4.549	1.676
Rmerge (all I+ & I-)	0.065	0.034	0.965
Rmeas (all I+ & I-)	0.071	0.037	1.046
Rpim (all I+ & I-)	0.027	0.015	0.400
Total number of observations	705031	35079	35256
Total number unique	106817	5677	5263
Mean(I)/sd(I)	14.6	37.1	2.2
Completeness	99.9	99.8	99.9
Multiplicity	6.6	6.2	6.7
CC(1/2)	0.999	0.999	0.857
Anomalous completeness	99.7	99.8	99.6
Anomalous multiplicity	3.4	3.4	3.4
CC(ano)	-0.111	-0.137	0.002
DANO /sd(DANO)	0.713	0.720	0.677

# Final scaling/merging - isotropic data analysis

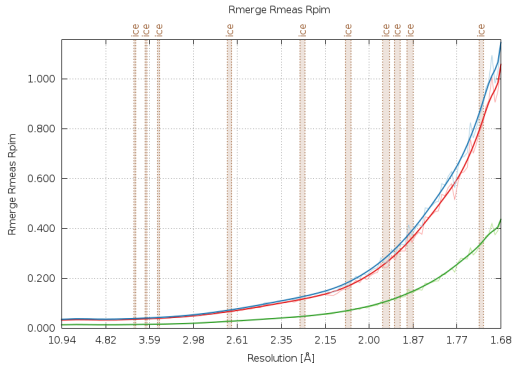


Fig.1 : R-values as a function of resolution

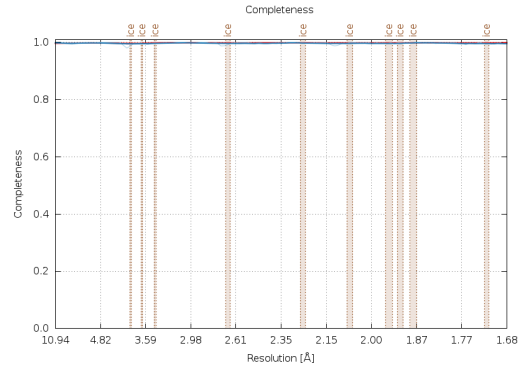


Fig.2 : Completeness as a function of resolution

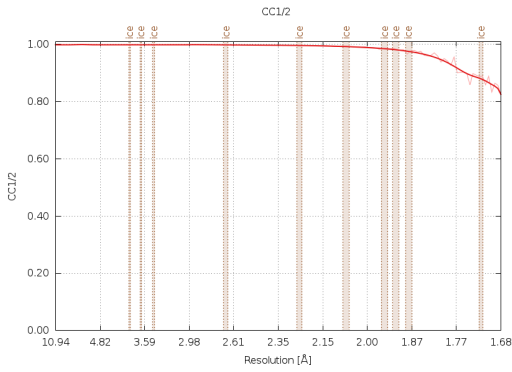


Fig.3 : CC1/2 as a function of resolution

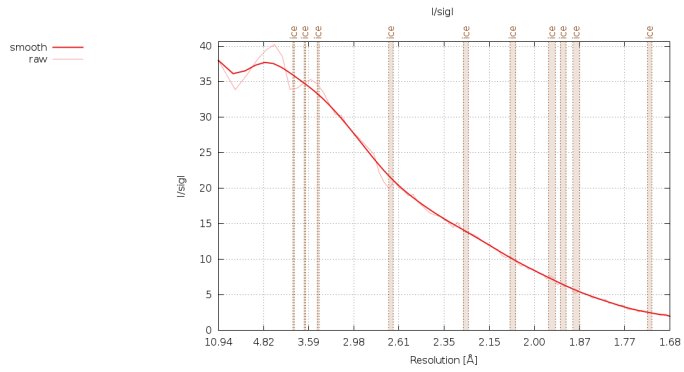


Fig.4 : I/sigI as a function of resolution

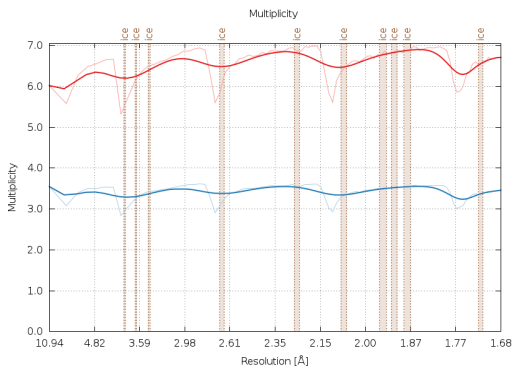


Fig.5 : Multiplicity as a function of resolution

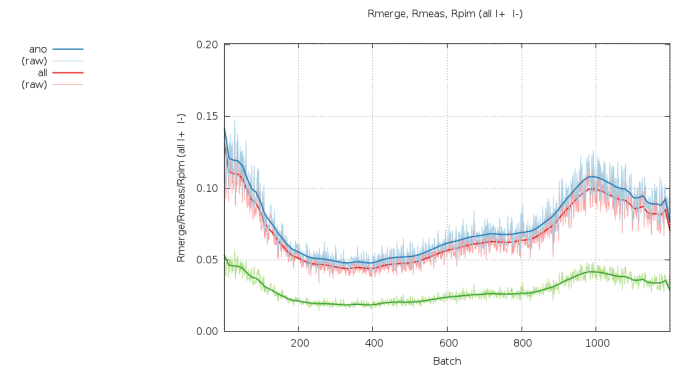


Fig.6 : R-values as a function of image number

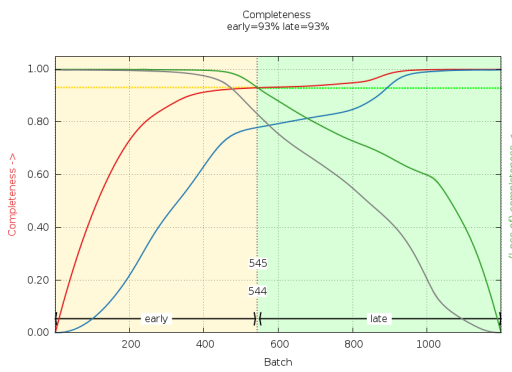


Fig.7 : Completeness as a function of image number

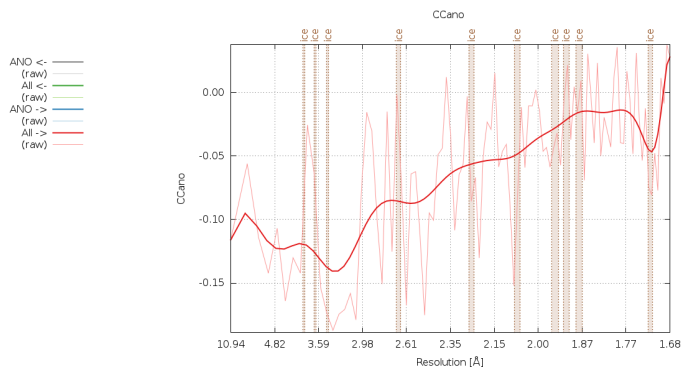
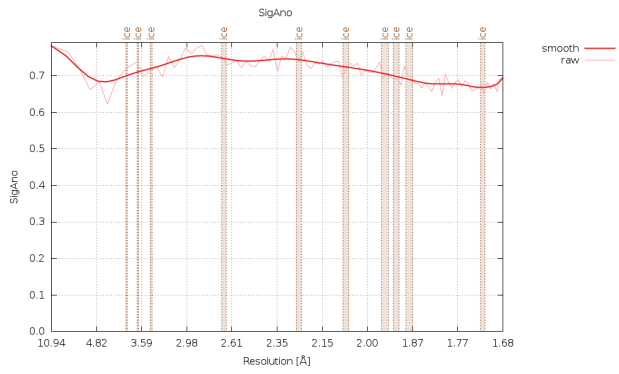
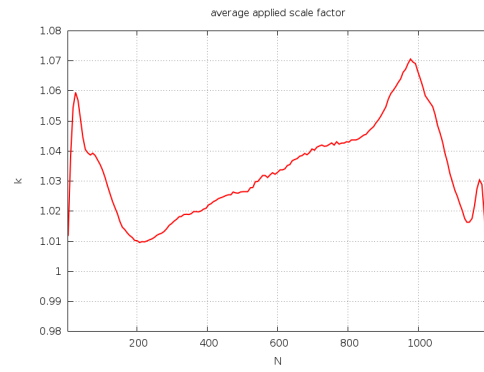


Fig.8 : CCano as a function of resolution

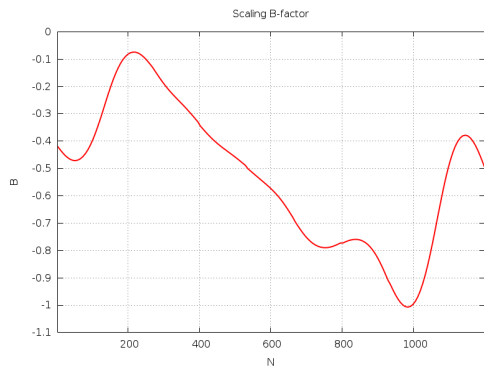
# Final scaling/merging - isotropic data analysis



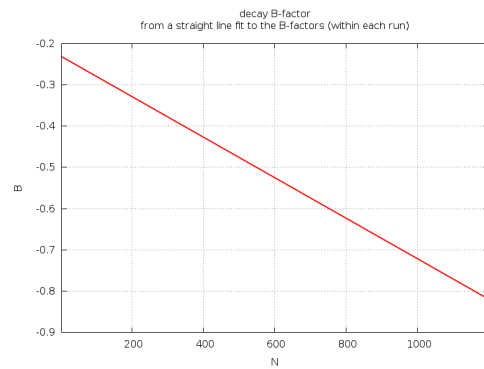
**Fig.9 :** SigAno as a function of resolution



**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

## 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. (2020). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.