

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 15:47:24 CEST 2020  
 autoPROC /home/software/xtal/GPhL/20200420  
 ADRP\_MPA\_M4\_F8\_eg\_data\_#####.cbf (1500 images, 375°)

Isotropic data analysis:

**Spacegroup** P21  
**Cell parameters** 37.177 33.174 60.612  
 90.000 96.181 90.000  
**Wavelength [Å]** 0.97918

	Overall	Inner Shell	Outer Shell
Low resolution limit	30.130	30.130	1.016
High resolution limit	0.999	2.712	0.999
Rmerge (all I+ & I-)	0.056	0.040	1.671
Rmeas (all I+ & I-)	0.060	0.044	1.973
Rpim (all I+ & I-)	0.023	0.017	1.024
Total number of observations	472052	27264	6263
Total number unique	73076	4079	1804
Mean(I)/sd(I)	13.9	37.5	0.8
Completeness	91.6	98.6	45.5
Multiplicity	6.5	6.7	3.5
CC(1/2)	0.998	0.997	0.382
Anomalous completeness	90.3	99.2	41.8
Anomalous multiplicity	3.3	3.5	1.8
CC(ano)	-0.299	-0.314	0.015
DANO /sd(DANO)	0.716	0.601	0.754

# Final scaling/merging - isotropic data analysis

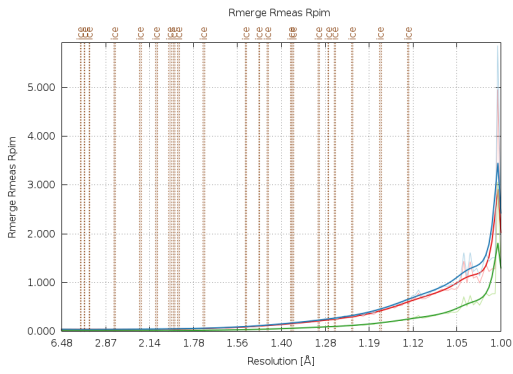


Fig.1 : R-values as a function of resolution

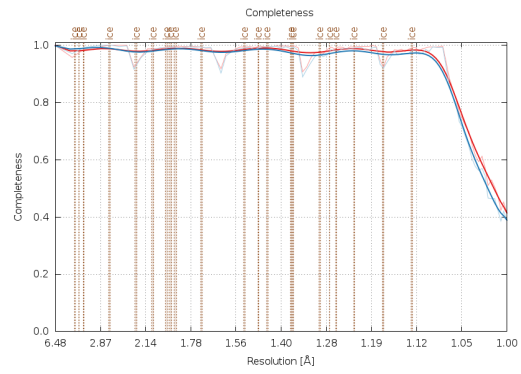


Fig.2 : Completeness as a function of resolution

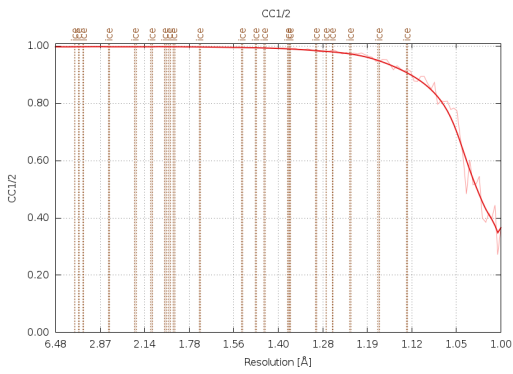


Fig.3 : CC1/2 as a function of resolution

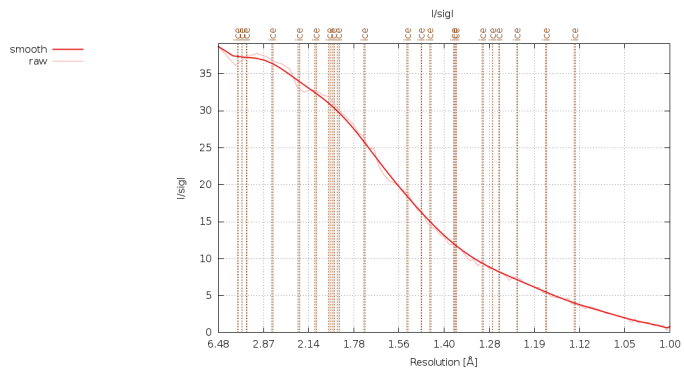


Fig.4 : I/sigI as a function of resolution

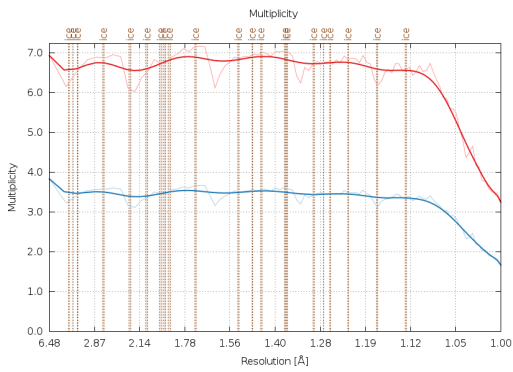


Fig.5 : Multiplicity as a function of resolution

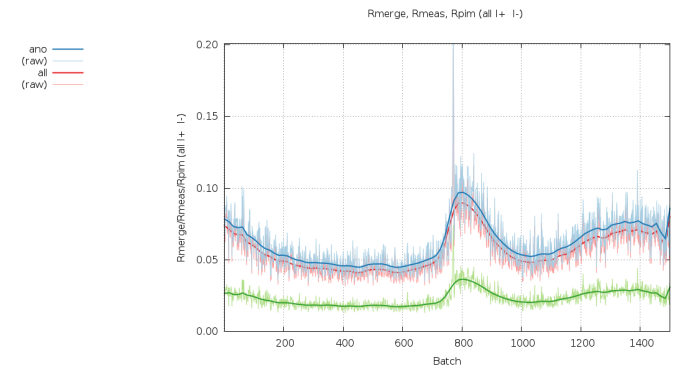


Fig.6 : R-values as a function of image number

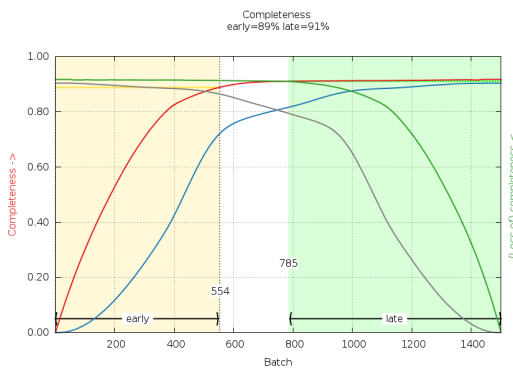


Fig.7 : Completeness as a function of image number

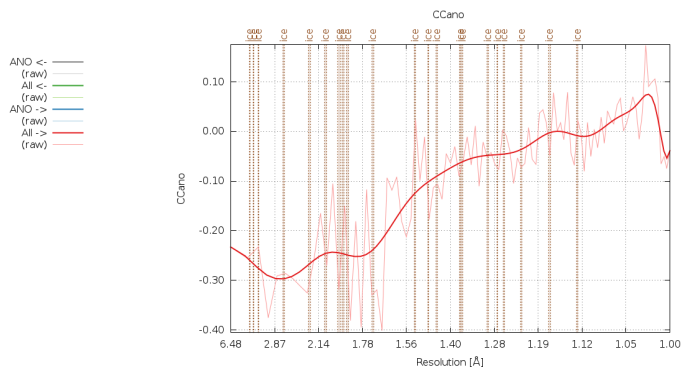
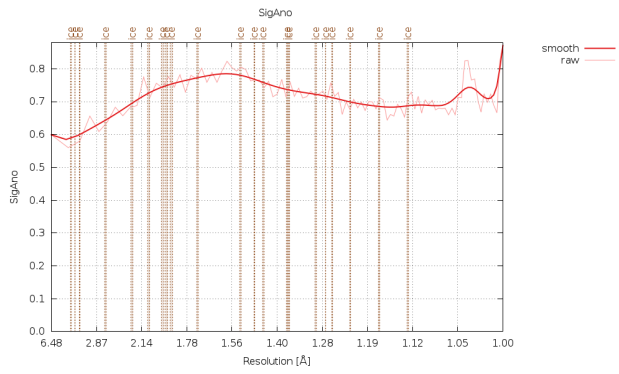
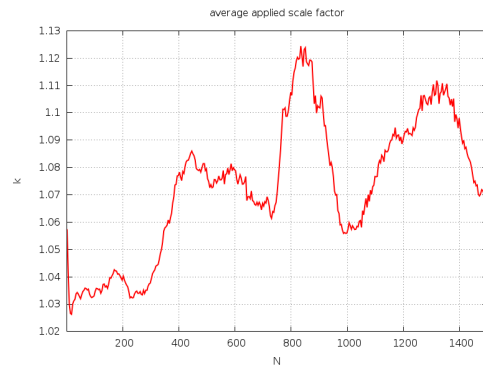


Fig.8 : CCano as a function of resolution

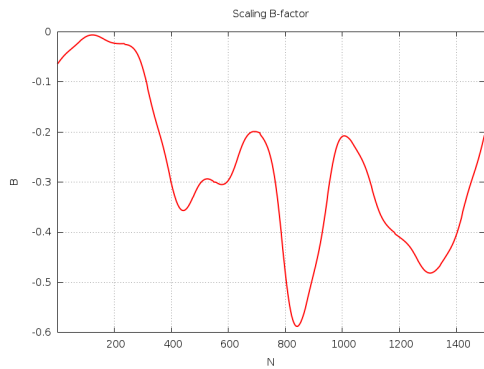
# Final scaling/merging - isotropic data analysis



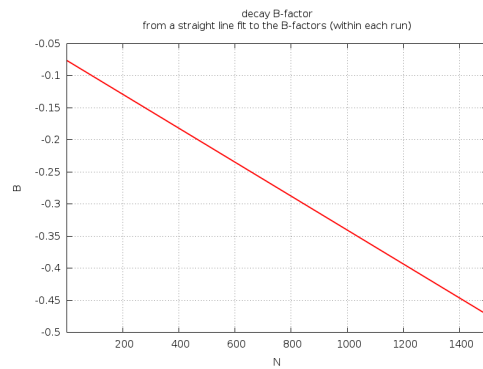
**Fig.9 :** SigAno as a function of resolution



**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.
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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.