

autoPROC 1.0.5 (20210716)  
XDS VERSION Jan 10, 2022 BUILT=20220220  
AIMLESS Version 0.7.7  
Host cn75  
User biomax-service (group = MAX-Lab)  
Date Fri Jul 1 23:29:44 CEST 2022  
autoPROC /mxn/groups/sw/mxsw/autoPROC  
HDF5\_1 MID2-x0504\_1\_1#####.h5 (1800 images, 360°)

### Isotropic data analysis:

Spacegroup P212121  
Cell parameters 54.114 61.064 119.673  
90.0 90.0 90.0  
Wavelength [Å] 0.97625

	Overall	Inner Shell	Outer Shell
Low resolution limit	54.392	54.392	1.942
High resolution limit	1.909	5.180	1.909
Rmerge (all I+ & I-)	0.053	0.028	1.321
Rmeas (all I+ & I-)	0.056	0.030	1.375
Rpim (all I+ & I-)	0.015	0.008	0.376
Total number of observations	397726	21402	13058
Total number unique	29759	1724	1014
Mean(I)/sd(I)	24.3	71.9	2.0
Completeness	94.3	99.9	66.1
Multiplicity	13.4	12.4	12.9
CC(1/2)	1.000	0.999	0.907
Anomalous completeness	94.0	100.0	65.0
Anomalous multiplicity	7.1	7.2	6.8
CC(ano)	-0.190	-0.216	0.054
DANO /sd(DANO)	0.737	0.796	0.672

## Final scaling/merging - isotropic data analysis

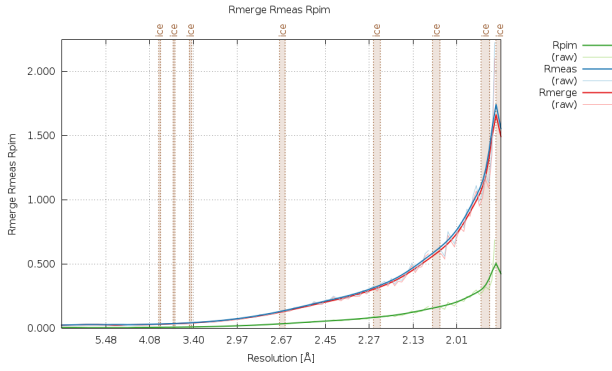


Fig.1 : R-values as a function of resolution

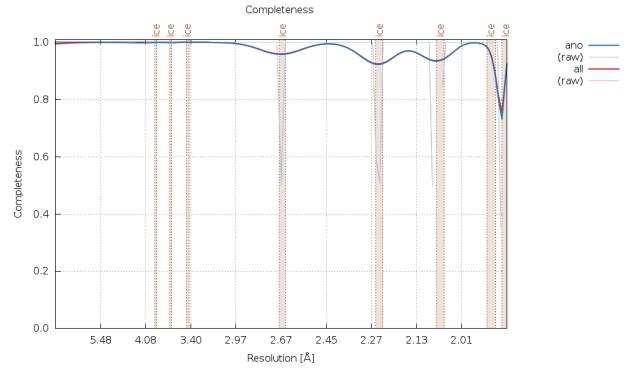


Fig.2 : Completeness as a function of resolution

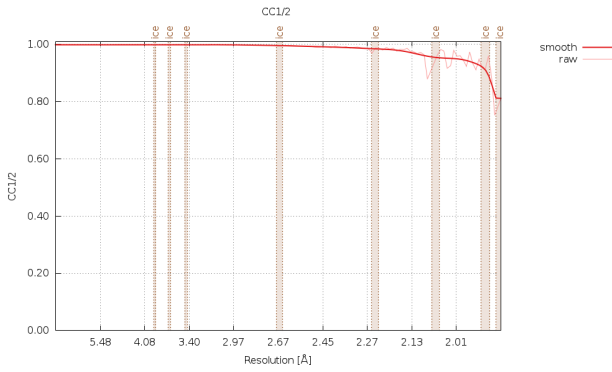


Fig.3 : CC1/2 as a function of resolution

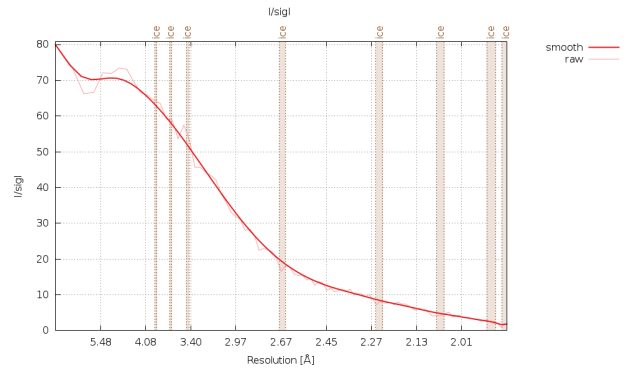


Fig.4 : I/sigI as a function of resolution

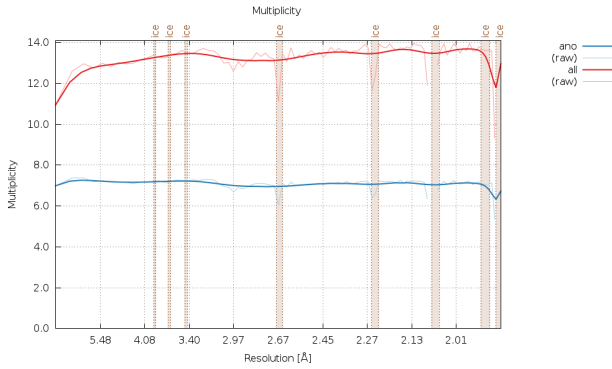


Fig.5 : Multiplicity as a function of resolution

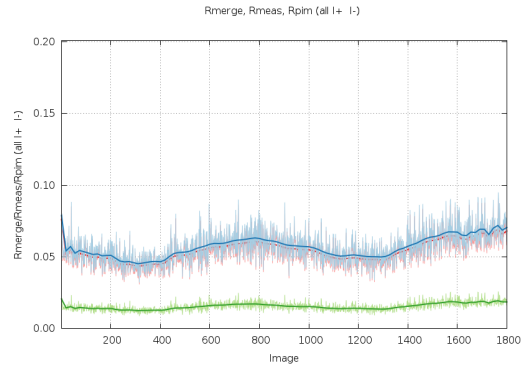


Fig.6 : R-values as a function of image number

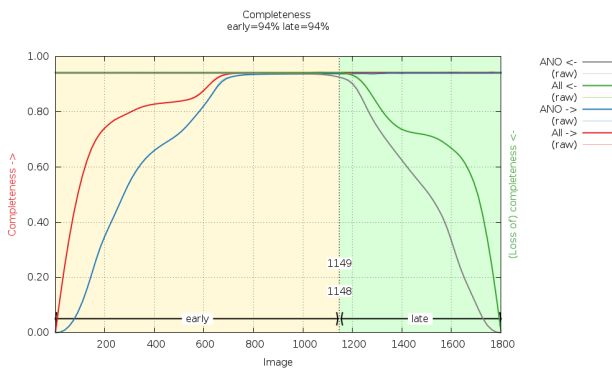


Fig.7 : Completeness as a function of image number

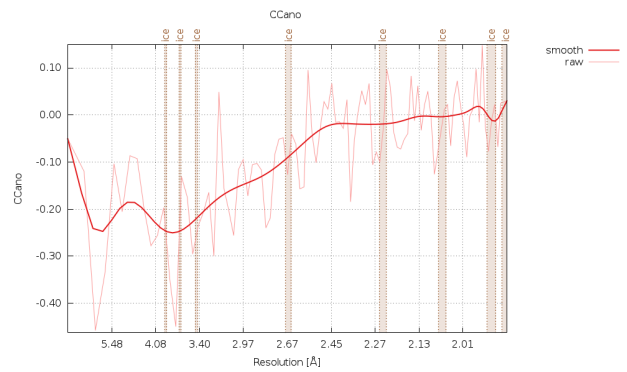
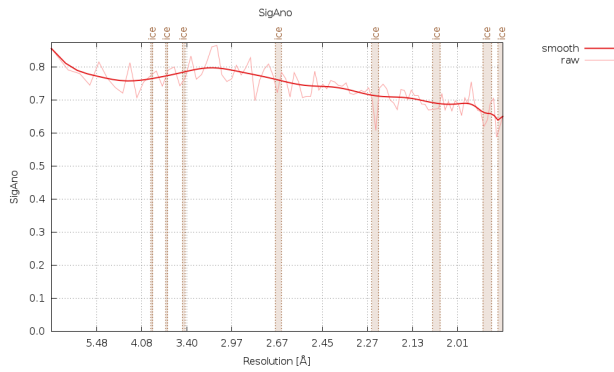
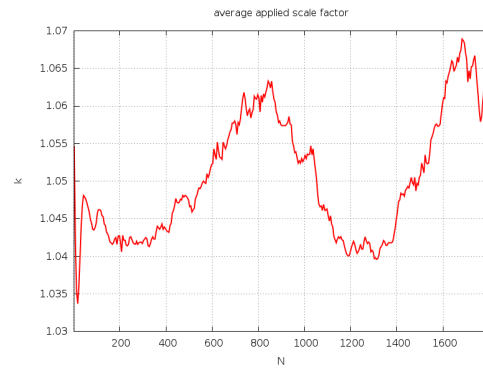


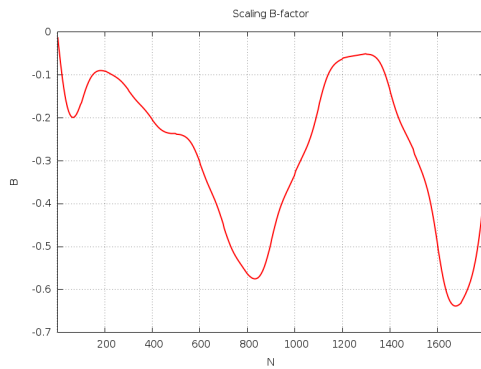
Fig.8 : CCano as a function of resolution



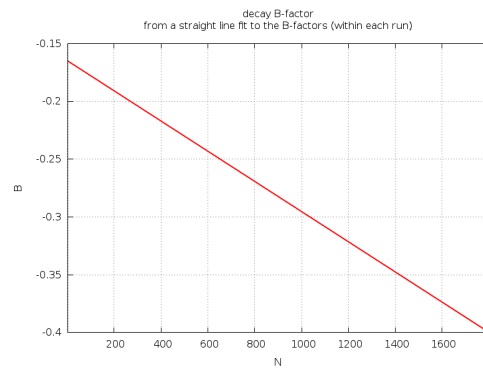
**Fig.9 :** SigAno as a function of resolution



**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. <i>Acta Cryst.</i> D67, 293-302.
XDS	Kabsch, W. (2010). XDS. <i>Acta Cryst.</i> D66, 125-132.
POINTLESS	Evans, P.R. (2006). Scaling and assessment of data quality, <i>Acta Cryst.</i> D62, 72-82.
AIMLESS	Evans, P.R. and Murshudov, G.N. (2013). How good are my data and what is the resolution?, <i>Acta Cryst.</i> 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, <i>Acta. Cryst.</i> D67, 235-242.
STARANISO	Tickle, I.J., Flensburg, C., Keller, P., Paciorek, W., Sharff, A., Vonrhein, C., and Bricogne, G. (2018-2021). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.