

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	Mon Apr 20 11:34:38 CEST 2020
autoPROC	/home/software/xtal/GPhL/20200420
	idp51000-201-a_1_2_3.### (195 images, 117°)

Isotropic data analysis:

Spacegroup	P3121
Cell parameters	167.722 167.722 51.941 90.0 90.0 120.0
Wavelength [Å]	0.97872
Anomalous signal up to	5.5 Å

	Overall	Inner Shell	Outer Shell
Low resolution limit	54.900	54.900	1.862
High resolution limit	1.831	4.969	1.831
Rmerge (all I+ & I-)	0.052	0.031	0.769
Rmeas (all I+ & I-)	0.056	0.033	0.827
Rpim (all I+ & I-)	0.020	0.012	0.303
Total number of observations	539775	26628	26964
Total number unique	73738	3850	3691
Mean(I)/sd(I)	20.5	50.8	2.3
Completeness	100.0	99.9	100.0
Multiplicity	7.3	6.9	7.3
CC(1/2)	0.999	0.999	0.812
Anomalous completeness	100.0	99.6	100.0
Anomalous multiplicity	3.8	3.7	3.7
CC(ano)	0.105	0.239	-0.003
DANO /sd(DANO)	0.786	1.142	0.650

Final scaling/merging - isotropic data analysis

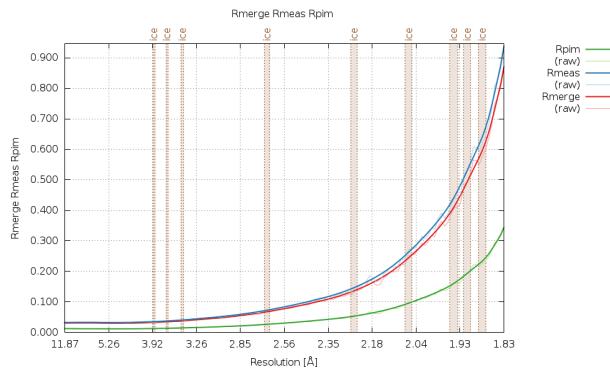


Fig.1 : R-values as a function of resolution

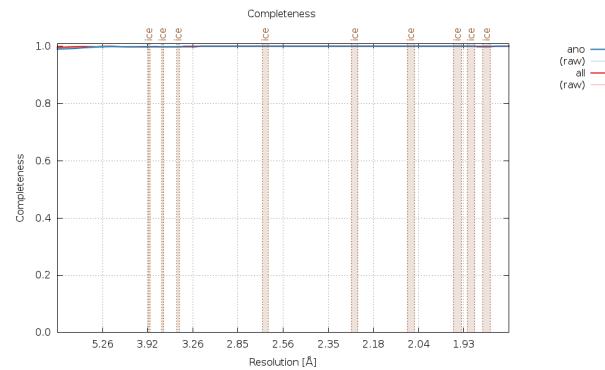


Fig.2 : Completeness as a function of resolution

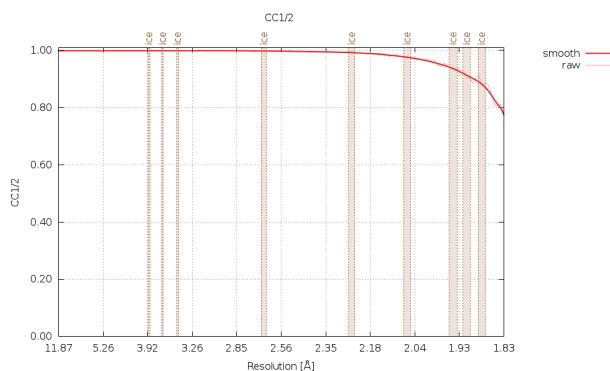


Fig.3 : CC1/2 as a function of resolution

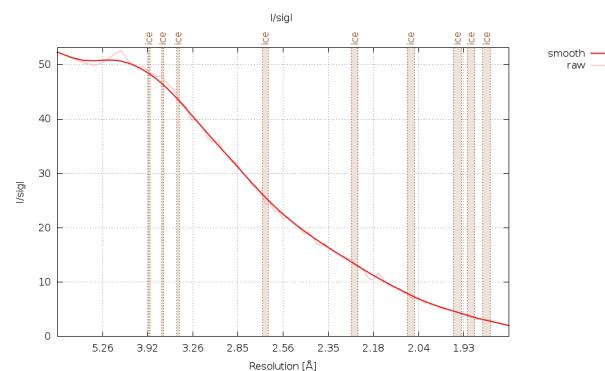


Fig.4 : I/sigl as a function of resolution

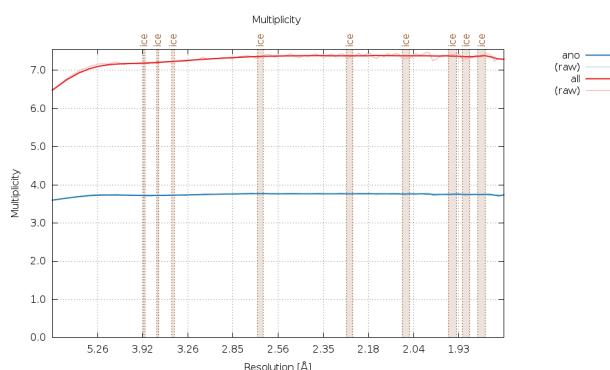


Fig.5 : Multiplicity as a function of resolution

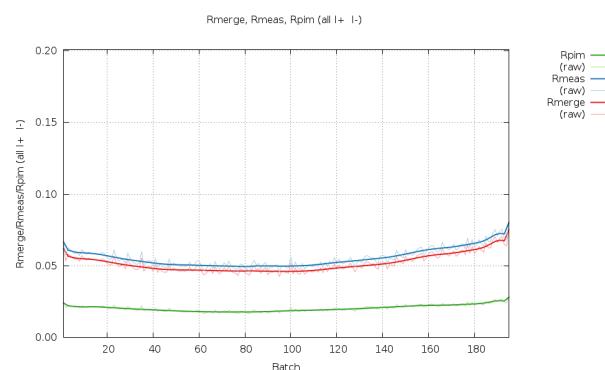


Fig.6 : R-values as a function of image number

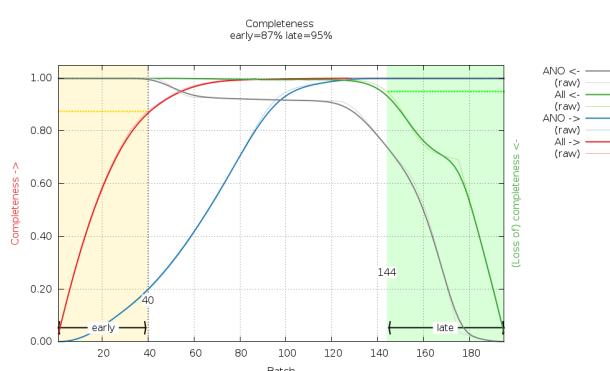


Fig.7 : Completeness as a function of image number

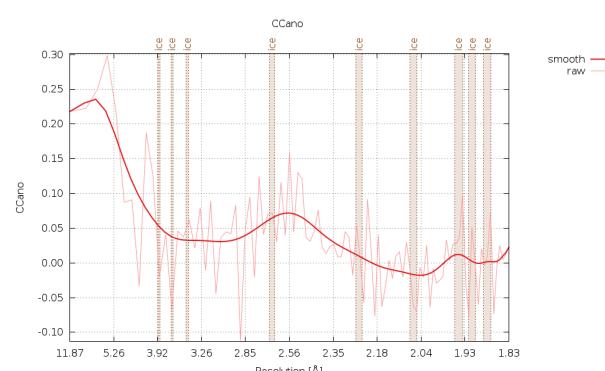


Fig.8 : CCano as a function of resolution

Final scaling/merging - isotropic data analysis

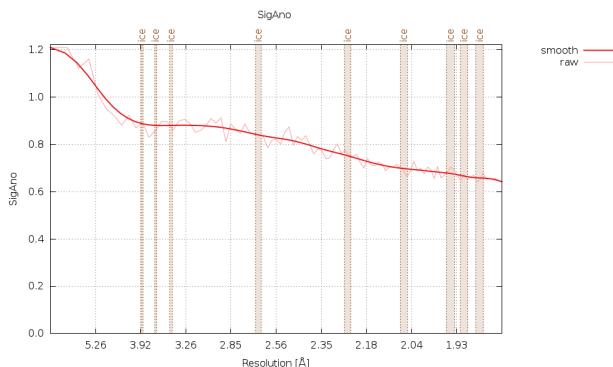


Fig.9 : SigAno as a function of resolution

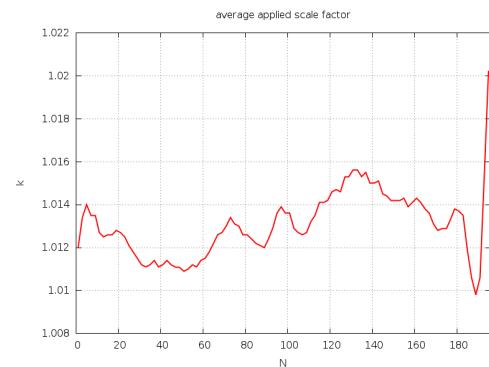


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

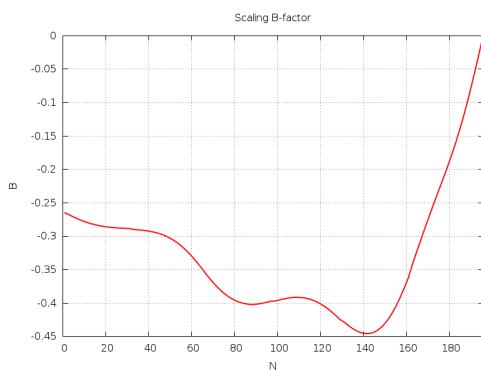


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

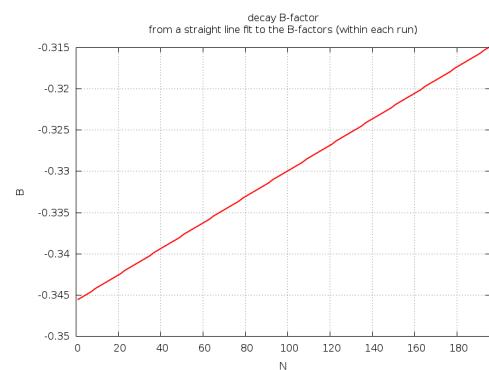


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

References

- 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.