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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 Thu Apr 23 11:23:42 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
Nsp15_M4_G4_RNA_eg_data_#####.cbf (180 images,
90°)
    
```

Isotropic data analysis:

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Spacegroup P63
Cell parameters 150.655 150.655 111.555
90.0 90.0 120.0
Wavelength [A] 0.97918
    
```

	Overall	Inner Shell	Outer Shell
Low resolution limit	45.103	45.103	1.971
High resolution limit	1.938	5.258	1.938
Rmerge (all I+ & I-)	0.075	0.036	1.036
Rmeas (all I+ & I-)	0.083	0.040	1.140
Rpim (all I+ & I-)	0.035	0.017	0.465
Total number of observations	542963	26950	27398
Total number unique	105220	5204	5272
Mean(I)/sd(I)	13.3	34.5	2.1
Completeness	98.8	95.5	99.4
Multiplicity	5.2	5.2	5.2
CC(1/2)	0.998	0.999	0.749
Anomalous completeness	90.8	89.7	91.6
Anomalous multiplicity	2.8	2.9	2.8
CC(ano)	-0.089	-0.179	-0.029
DANO /sd(DANO)	0.770	0.779	0.698

# Final scaling/merging - isotropic data analysis

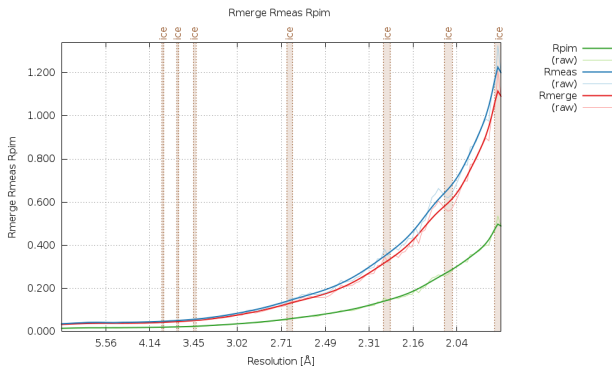


Fig.1 : R-values as a function of resolution

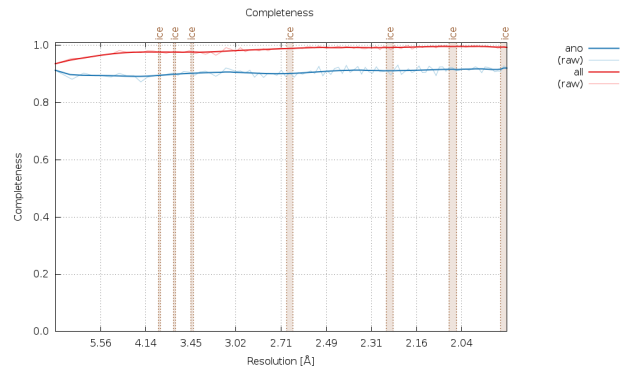


Fig.2 : Completeness as a function of resolution

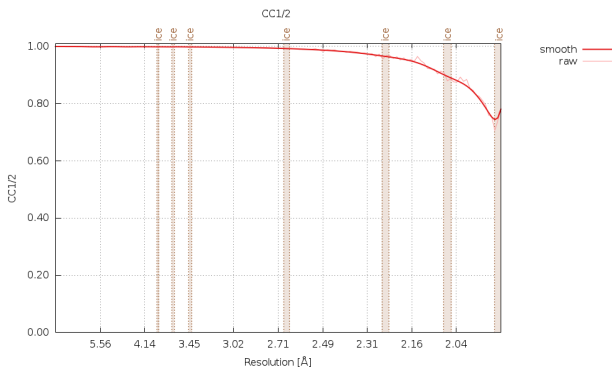


Fig.3 : CC1/2 as a function of resolution

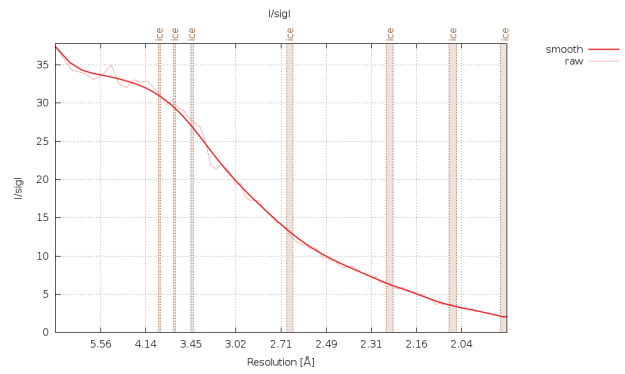


Fig.4 : I/sigI as a function of resolution

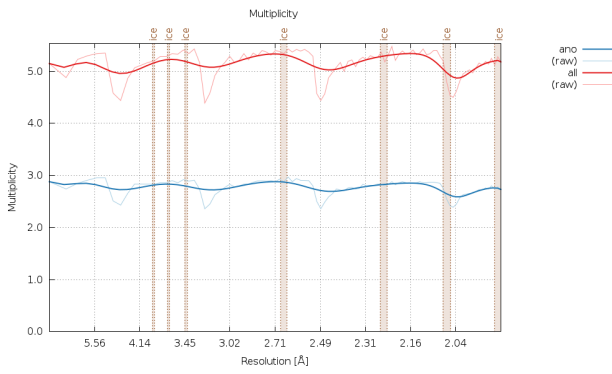


Fig.5 : Multiplicity as a function of resolution

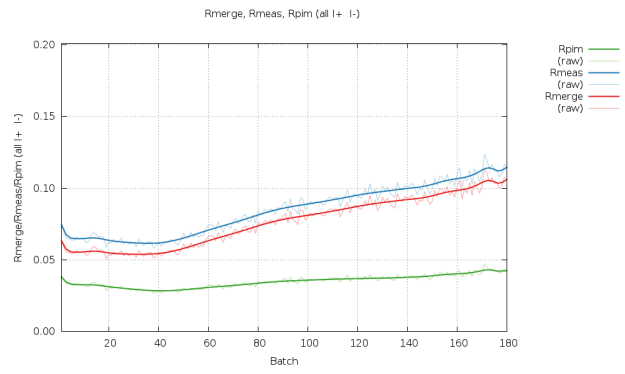


Fig.6 : R-values as a function of image number

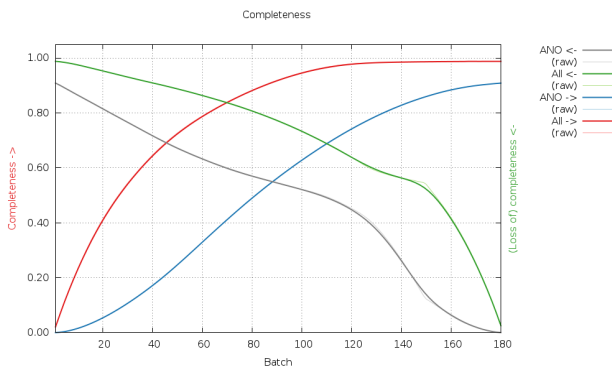


Fig.7 : Completeness as a function of image number

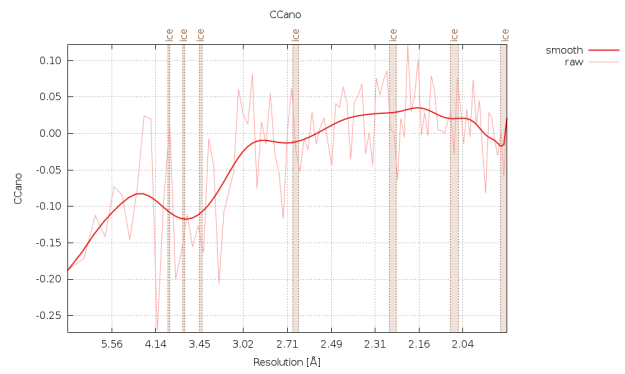


Fig.8 : CCano as a function of resolution

# Final scaling/merging - isotropic data analysis

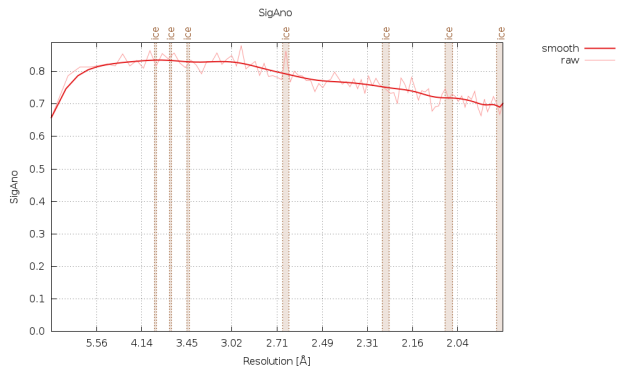


Fig.9 : SigAno as a function of resolution

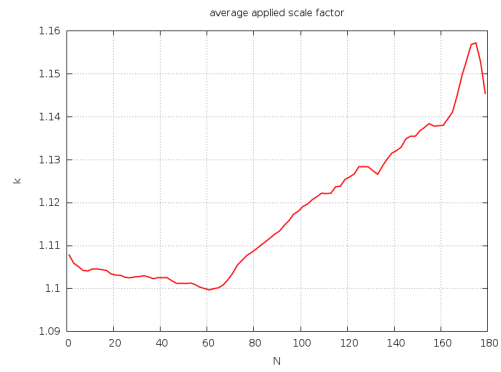


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

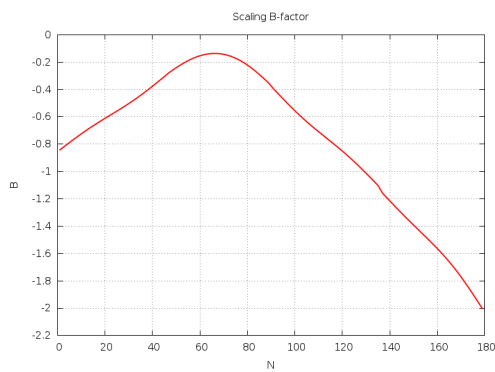


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

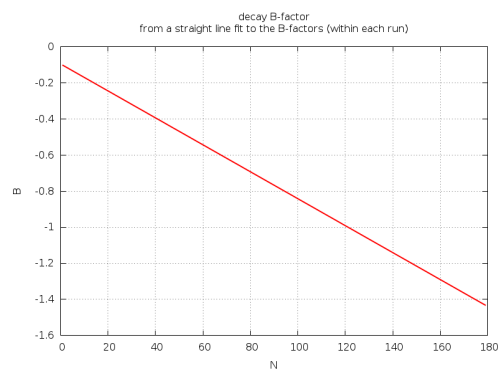


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

## 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.