

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 | 1.941 |
| High resolution limit | 1.908 | 5.178 | 1.908 |
| Rmerge (all I+ & I-) | 0.053 | 0.028 | 1.360 |
| Rmeas (all I+ & I-) | 0.055 | 0.029 | 1.416 |
| Rpim (all I+ & I-) | 0.015 | 0.008 | 0.388 |
| Total number of observations | 398350 | 21446 | 13254 |
| Total number unique | 29816 | 1726 | 1030 |
| Mean(I)/sd(I) | 24.5 | 72.9 | 2.0 |
| Completeness | 94.3 | 99.9 | 66.5 |
| Multiplicity | 13.4 | 12.4 | 12.9 |
| CC(1/2) | 1.000 | 0.999 | 0.899 |
| Anomalous completeness | 94.0 | 99.9 | 65.2 |
| Anomalous multiplicity | 7.1 | 7.3 | 6.8 |
| CC(ano) | -0.093 | -0.086 | 0.071 |
| DANO /sd(DANO) | 0.786 | 0.910 | 0.673 |

Final scaling/merging - isotropic data analysis

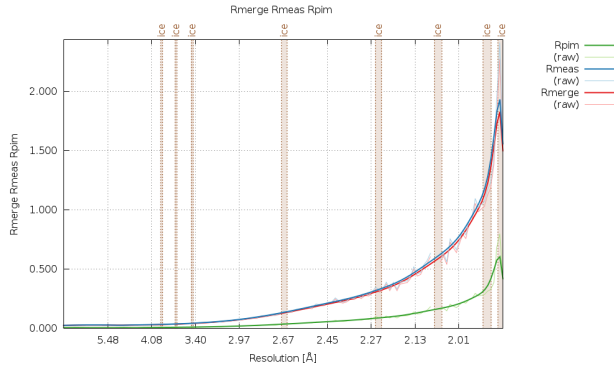


Fig.1 : R-values as a function of resolution

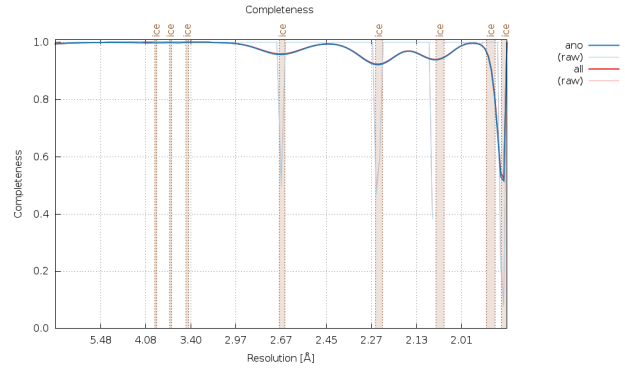


Fig.2 : Completeness as a function of resolution

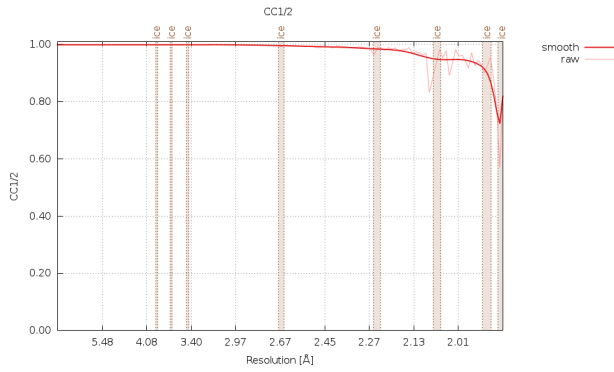


Fig.3 : CC1/2 as a function of resolution

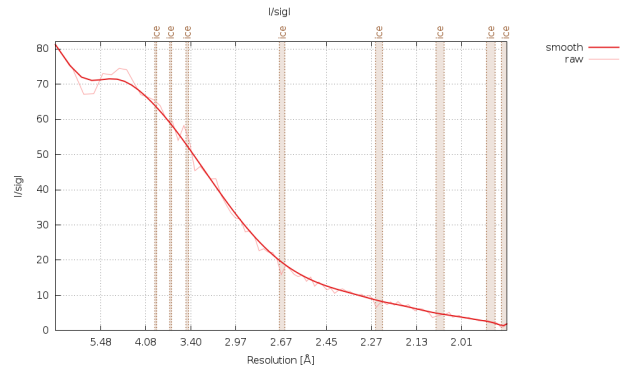


Fig.4 : I/sigI as a function of resolution

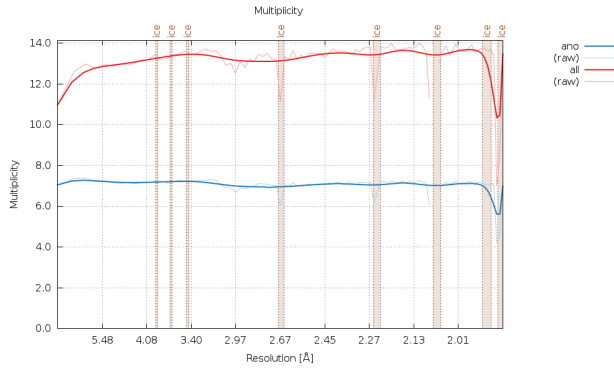


Fig.5 : Multiplicity as a function of resolution

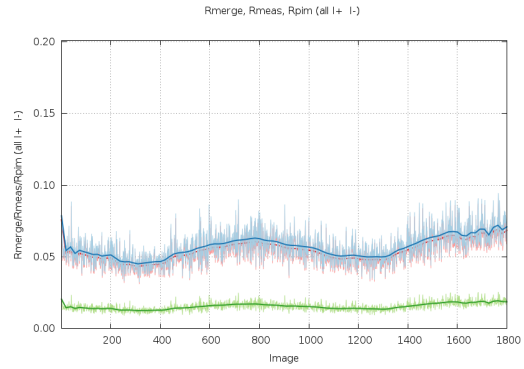


Fig.6 : R-values as a function of image number

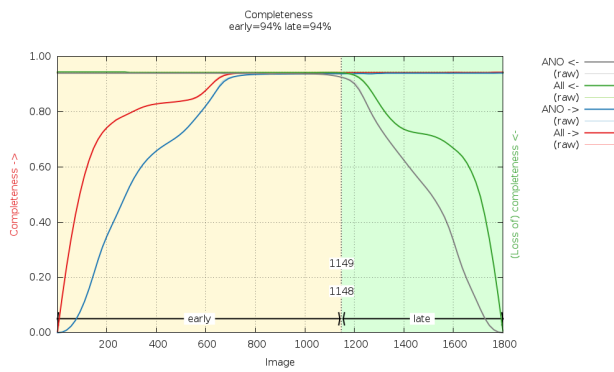


Fig.7 : Completeness as a function of image number

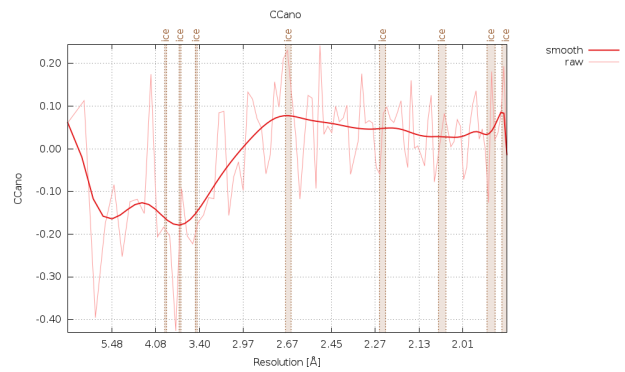


Fig.8 : CCano as a function of resolution

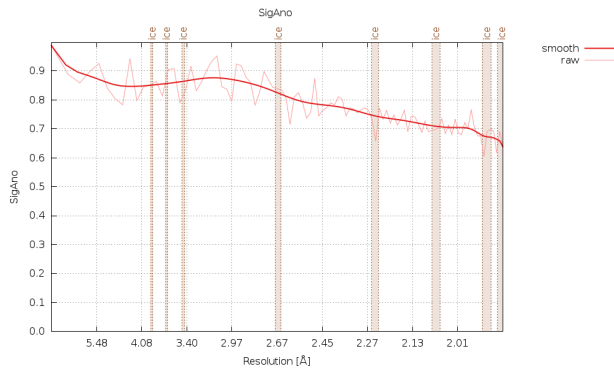


Fig.9 : SigAno as a function of resolution

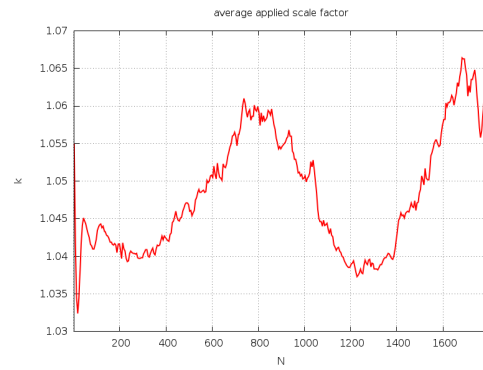


Fig.10 : Scale factor (AIMLESS scaling) as a function of image number

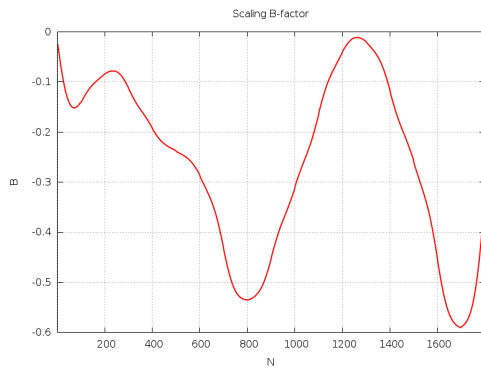


Fig.11 : Scaling B-factor (AIMLESS scaling) as a function of image number

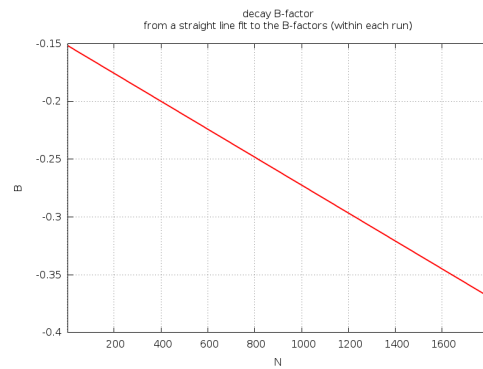


Fig.12 : Decay B-factor (AIMLESS scaling) as a function of image number

References

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| 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. |