

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°)

Anisotropic data analysis with STARANISO:

Spacegroup P212121
Cell parameters 54.114 61.064 119.673
90.0 90.0 90.0
Wavelength [Å] 0.97625
Diffraction limits [Å] 1.999 1.845 1.601
Eigenvector-1 1.000 0.000 0.000
Eigenvector-2 0.000 1.000 0.000
Eigenvector-3 0.000 0.000 1.000
Direction-1 a_*
Direction-2 b_*
Direction-3 c_*

	Overall	Inner Shell	Outer Shell
Low resolution limit	54.392	54.392	1.794
High resolution limit	1.609	5.240	1.609
Rmerge (all I+ & I-)	0.055	0.028	1.381
Rmeas (all I+ & I-)	0.057	0.030	1.443
Rpim (all I+ & I-)	0.016	0.008	0.414
Total number of observations	443158	20709	20201
Total number unique	33460	1672	1674
Mean(I)/sd(I)	20.8	66.2	1.8
Completeness (spherical)	64.0	99.9	11.6
Completeness (ellipsoidal)	90.0	99.9	68.7
Multiplicity	13.2	12.4	12.1
CC(1/2)	1.000	0.999	0.750
Anomalous completeness (spherical)	62.6	100.0	10.6
Anomalous completeness (ellipsoidal)	89.5	100.0	66.5
Anomalous multiplicity	7.0	7.2	6.4
CC(ano)	-0.176	-0.085	-0.023
DANO /sd(DANO)	0.719	0.739	0.682

Final scaling/merging - anisotropic data analysis via STARANISO

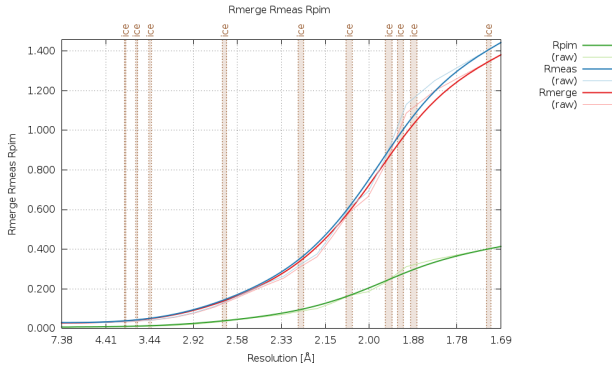


Fig.1 : R-values as a function of resolution (observations)

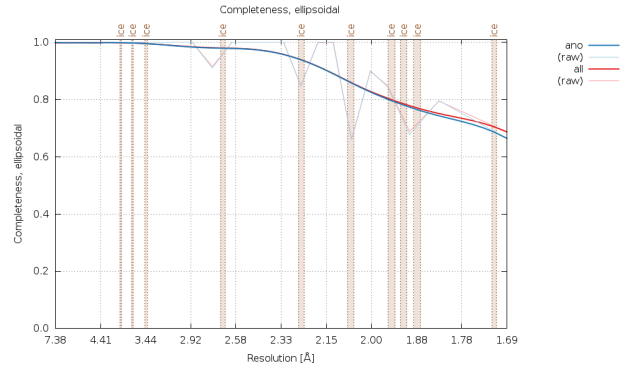


Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.

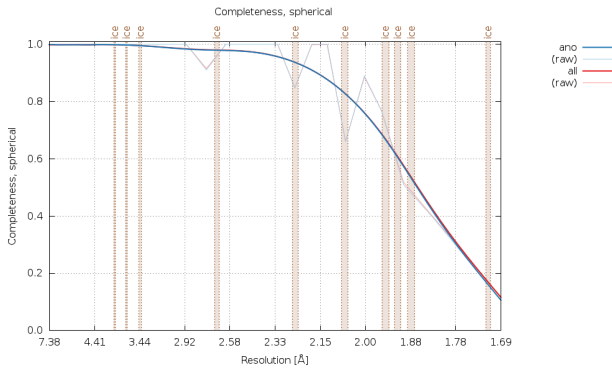


Fig.3 : Completeness (spherical) as a function of resolution (observations)

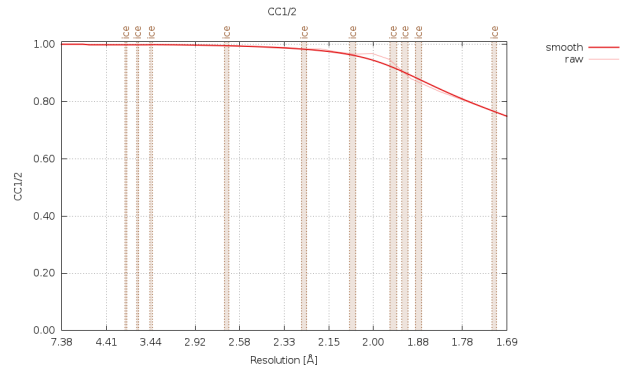


Fig.4 : CC1/2 as a function of resolution (observations)

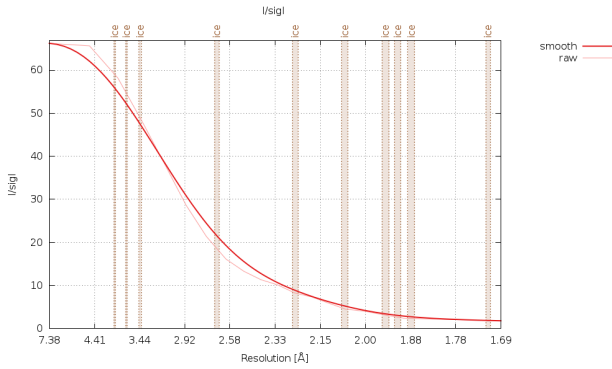


Fig.5 : I/sigI as a function of resolution (observations)

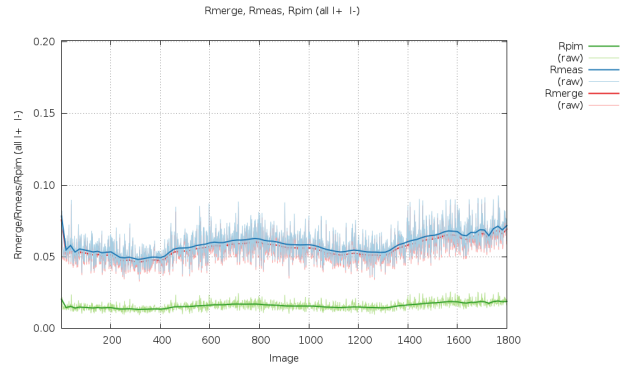


Fig.6 : R-values as a function of image number (observations)

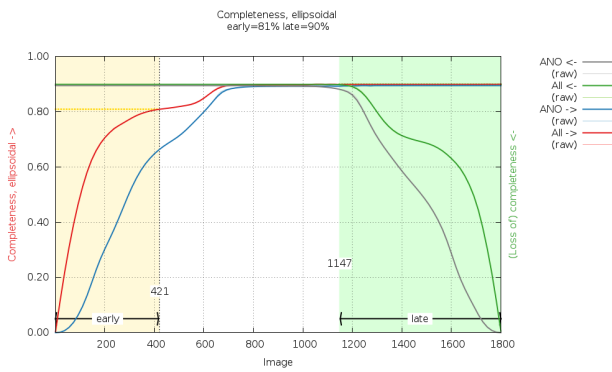


Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.

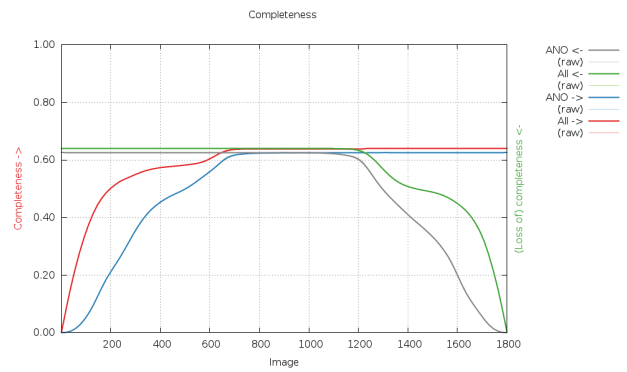


Fig.8 : Completeness (spherical) as a function of image number (observations)

Final scaling/merging - anisotropic data analysis via STARANISO

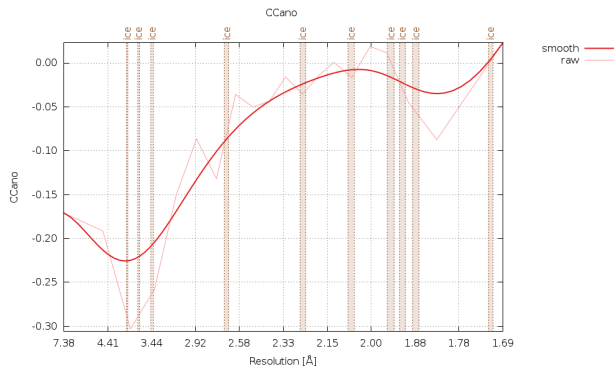


Fig.9 : CCano as a function of resolution (observations)

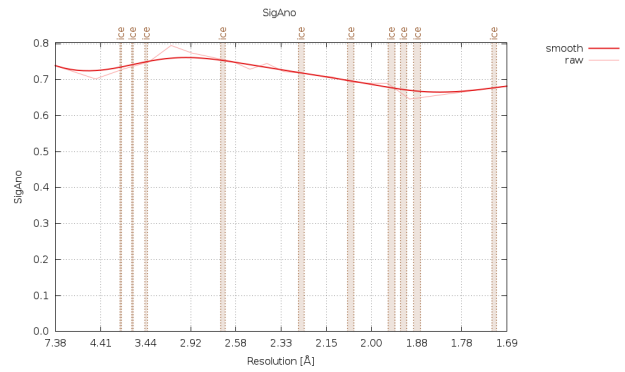


Fig.10 : SigAno as a function of resolution (observations)

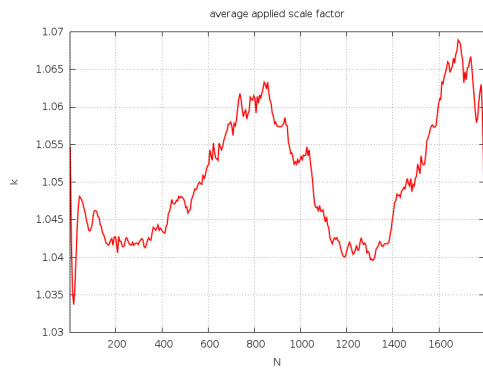


Fig.11 : Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

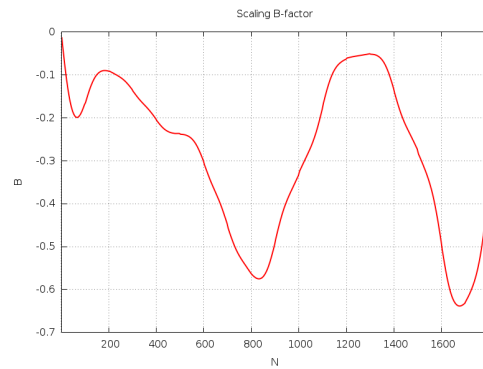


Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

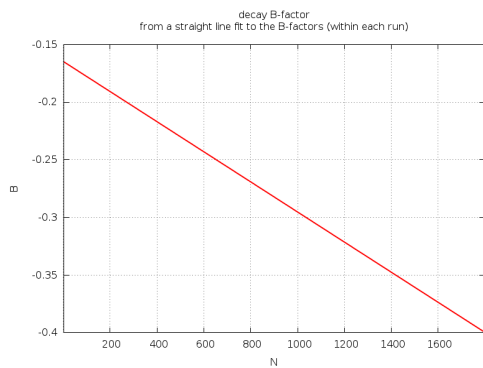


Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

Final scaling/merging - anisotropic data analysis via STARANISO (all measurements - for comparison only)

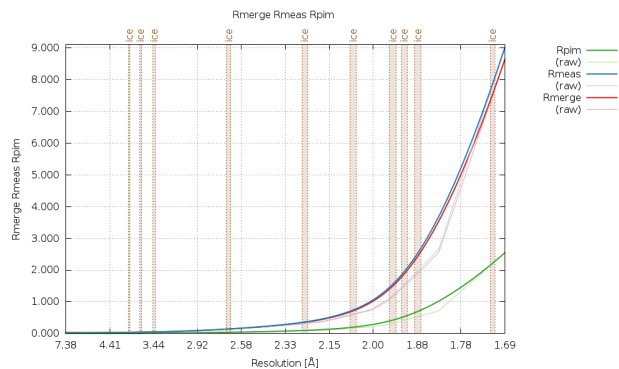


Fig.14 : R-values as a function of resolution (measurements)

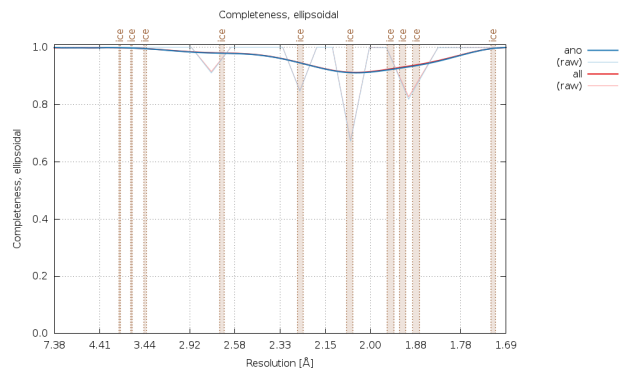


Fig.15 : Completeness (ellipsoidal) as a function of resolution (measurements)

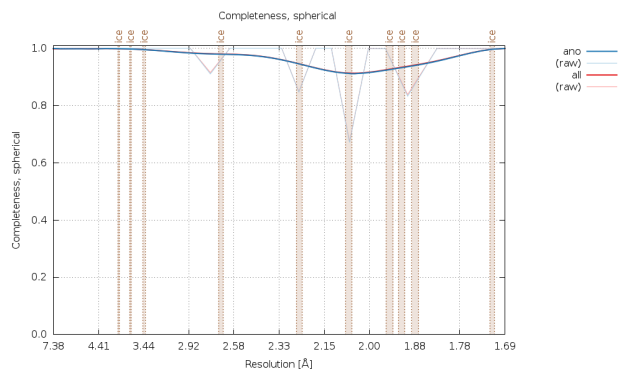


Fig.16 : Completeness (spherical) as a function of resolution (measurements)

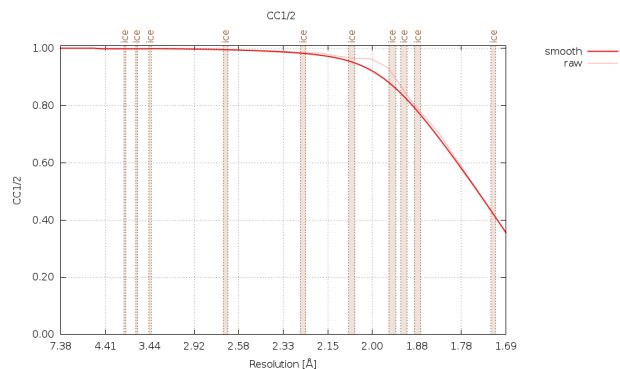


Fig.17 : CC1/2 as a function of resolution (measurements)

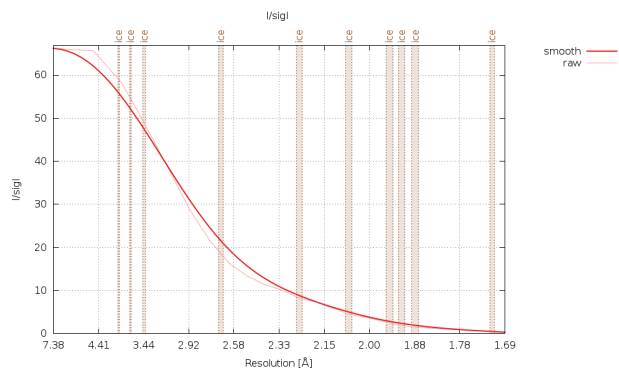


Fig.18 : I/sigI as a function of resolution (measurements)

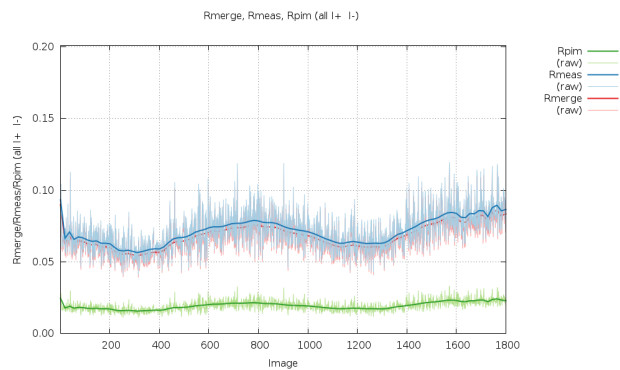


Fig.19 : R-values as a function of image number (measurements)

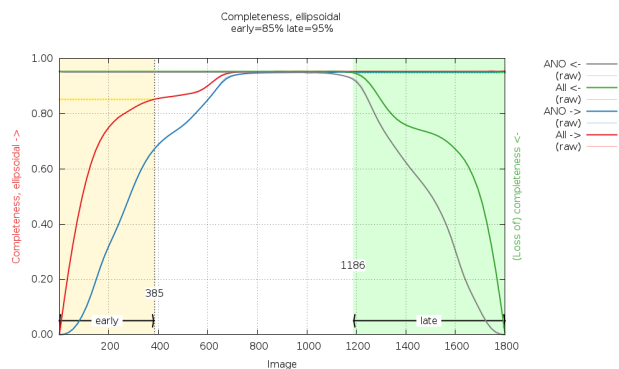


Fig.20 : Completeness (ellipsoidal) as a function of image number (measurements)

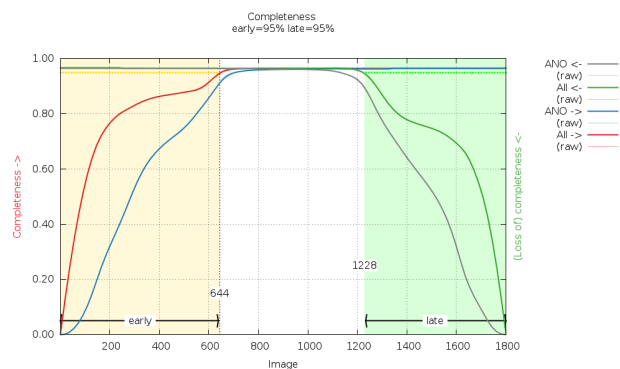


Fig.21 : Completeness (spherical) as a function of image number (measurements)

Final scaling/merging - anisotropic data analysis via STARANISO (all measurements - for comparison only)

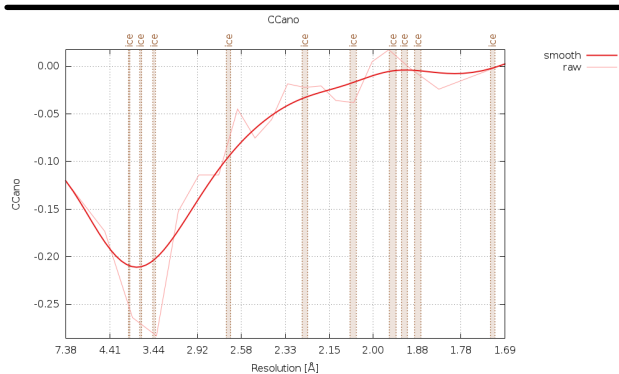


Fig.22 : CCano as a function of resolution (measurements)

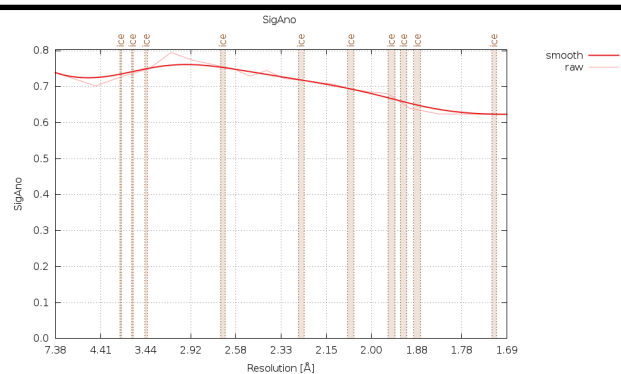


Fig.23 : SigAno as a function of resolution (measurements)

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. <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.