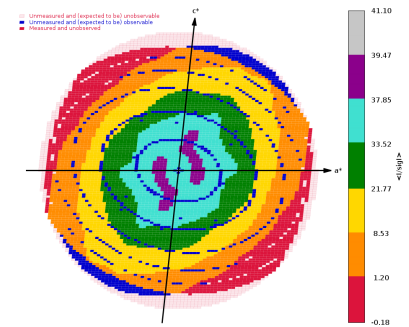
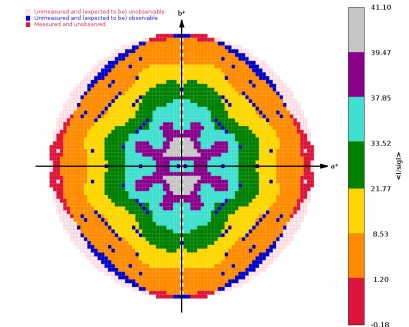


STARANISO local <I/sig> H=0 plane



STARANISO local <I/sig> K=0 plane



STARANISO local <I/sig> L=0 plane

```

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 Fri Apr 24 15:47:24 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
ADRP_MPA_M4_F8_eg_data_#####.cbf (1500 images,
375°)
    
```

Anisotropic data analysis with STARANISO:

```

Spacegroup P21
Cell parameters 37.177 33.174 60.612
90.000 96.181 90.000
Wavelength [A] 0.97918
Diffraction limits [A] 1.176 0.971 0.960
Eigenvector-1 0.773 0.000 -0.634
Eigenvector-2 0.000 1.000 0.000
Eigenvector-3 0.634 0.000 0.773
Direction-1 0.553 _a_* - 0.833 _c_*
Direction-2 _b_*
Direction-3 0.486 _a_* + 0.874 _c_*
    
```

	Overall	Inner Shell	Outer Shell
Low resolution limit	30.130	30.130	1.031
High resolution limit	0.960	2.898	0.960
Rmerge (all I+ & I-)	0.054	0.040	1.008
Rmeas (all I+ & I-)	0.059	0.044	1.175
Rpim (all I+ & I-)	0.022	0.017	0.588
Total number of observations	436570	22167	12554
Total number unique	66917	3344	3347
Mean(I)/sd(I)	15.2	37.6	1.4
Completeness (spherical)	74.6	98.3	19.5
Completeness (ellipsoidal)	90.9	98.3	48.1
Multiplicity	6.5	6.6	3.8
CC(1/2)	0.998	0.997	0.400
Anomalous completeness (spherical)	73.6	99.0	18.2
Anomalous completeness (ellipsoidal)	89.9	99.0	44.9
Anomalous multiplicity	3.4	3.5	2.0
CC(ano)	-0.304	-0.321	0.077
DANO /sd(DANO)	0.728	0.603	0.782

Final scaling/merging - anisotropic data analysis via STARANISO

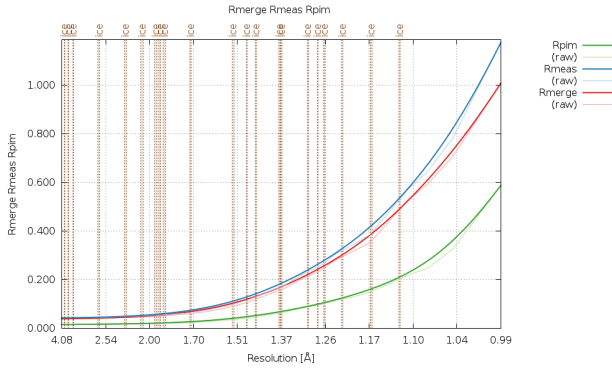


Fig.1 : R-values as a function of resolution (observations)

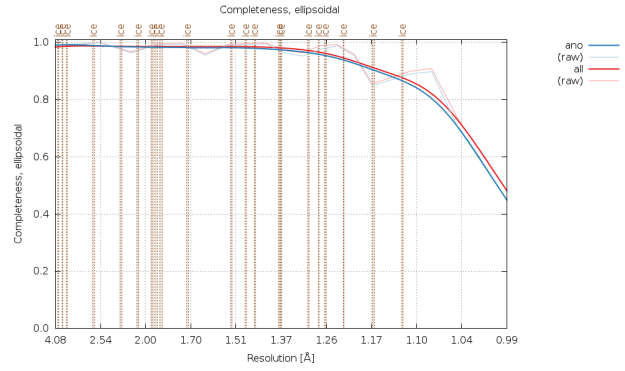


Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.

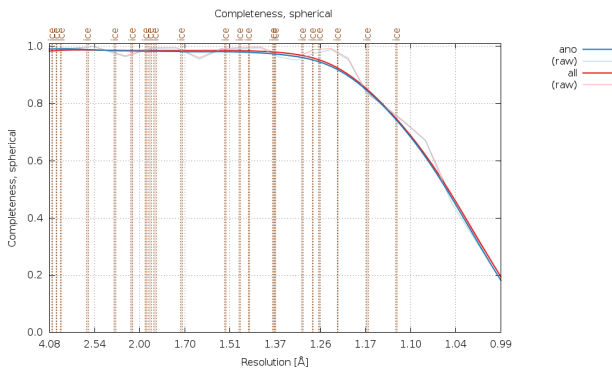


Fig.3 : Completeness (spherical) as a function of resolution (observations)

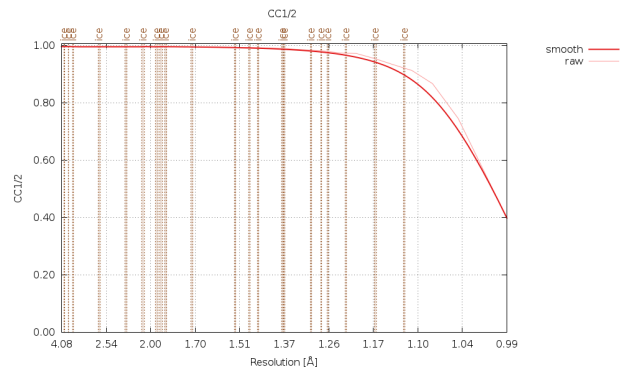


Fig.4 : CC1/2 as a function of resolution (observations)

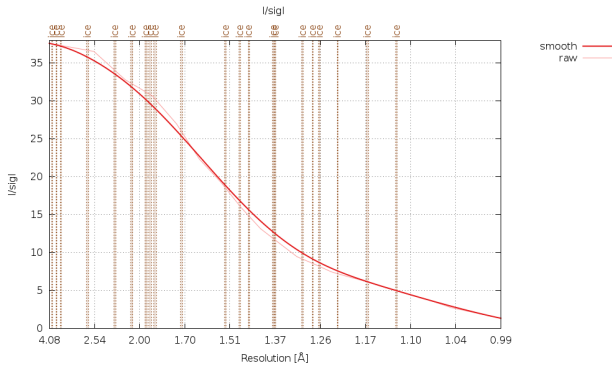


Fig.5 : I/sigI as a function of resolution (observations)

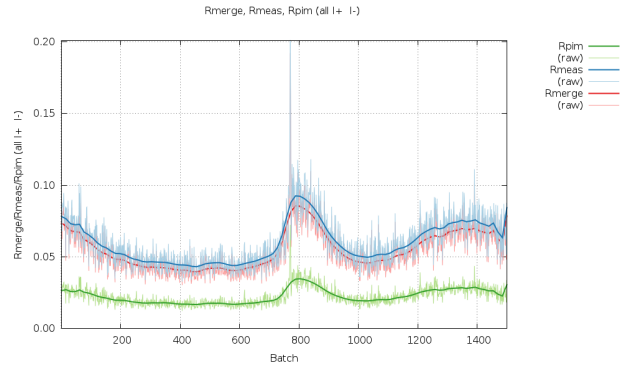


Fig.6 : R-values as a function of image number (observations)

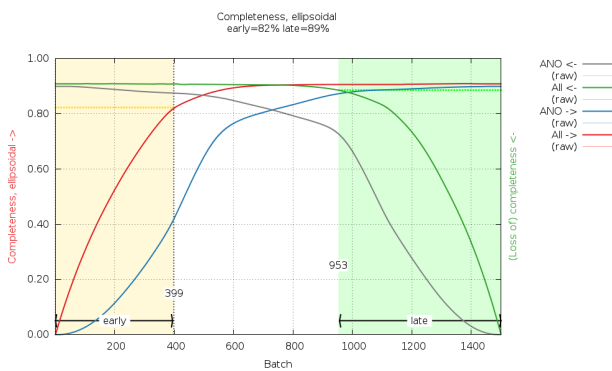


Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.

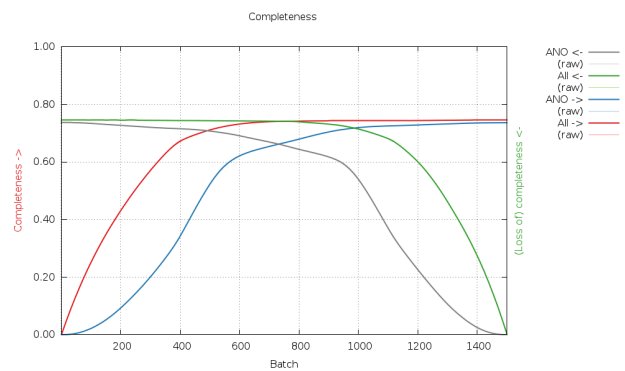


Fig.8 : Completeness (spherical) as a function of image number (observations)

Final scaling/merging - anisotropic data analysis via STARANISO

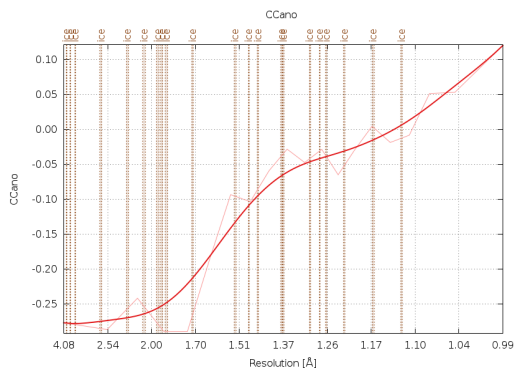


Fig.9 : CCano as a function of resolution (observations)

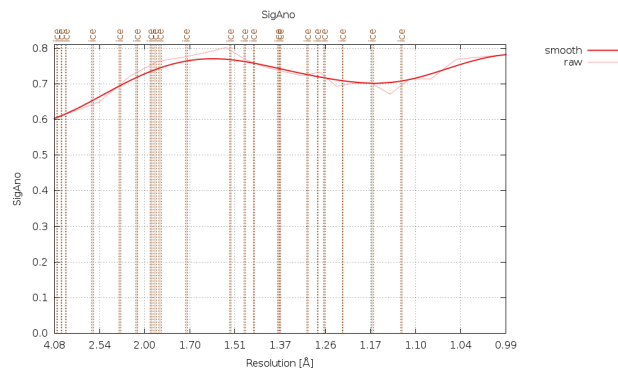


Fig.10 : SigAno as a function of resolution (observations)

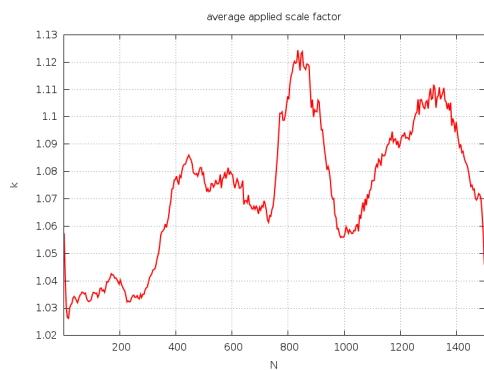


Fig.11 : Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

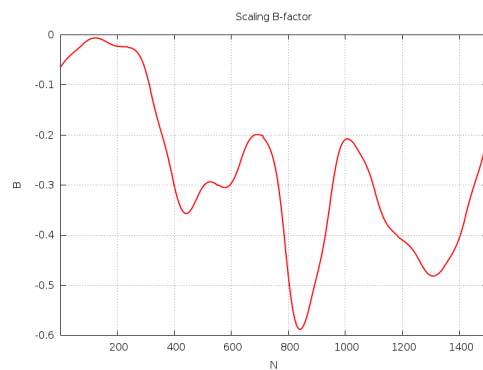


Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

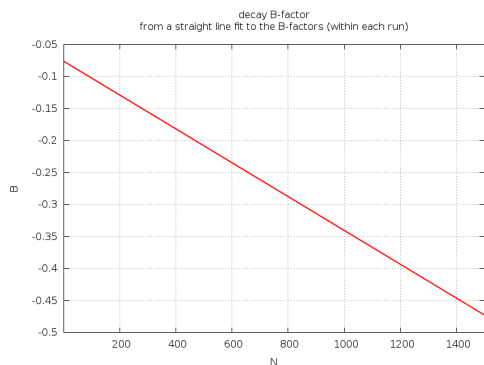


Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

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

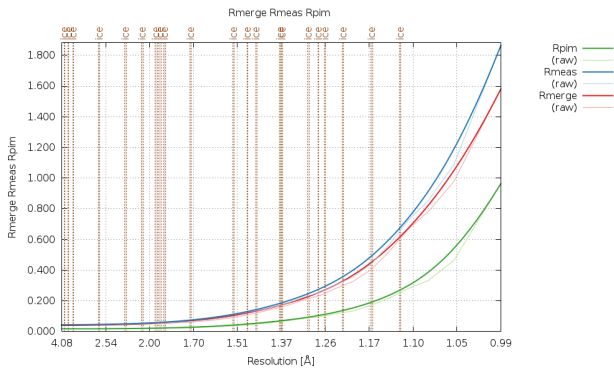


Fig.14 : R-values as a function of resolution (measurements)

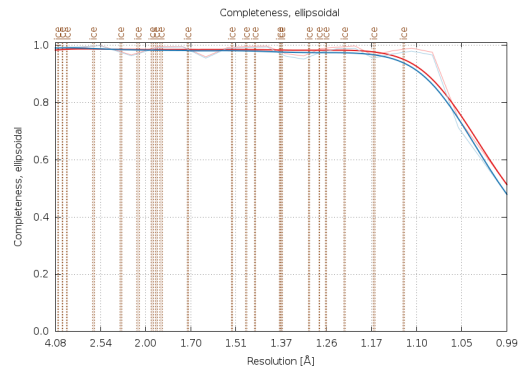


Fig.15 : Completeness (ellipsoidal) as a function of resolution (measurements)

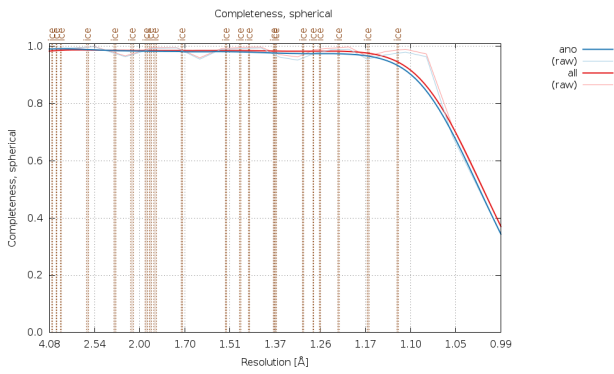


Fig.16 : Completeness (spherical) as a function of resolution (measurements)

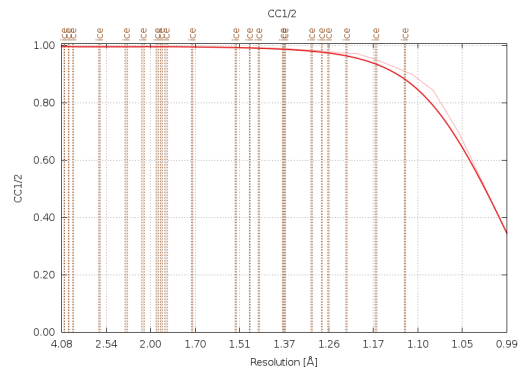


Fig.17 : CC1/2 as a function of resolution (measurements)

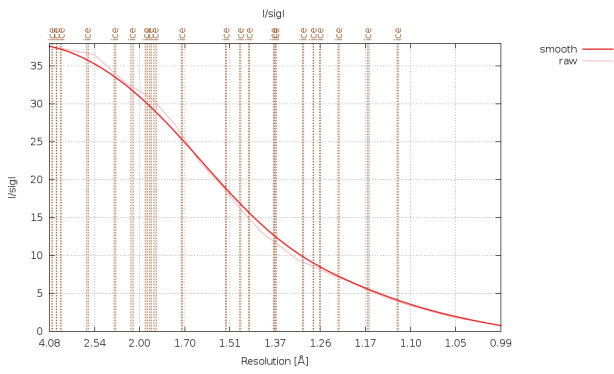


Fig.18 : I/sigI as a function of resolution (measurements)

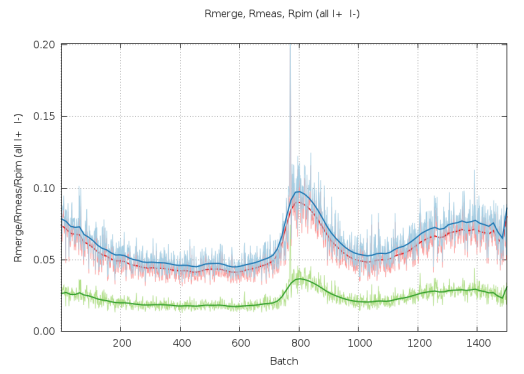


Fig.19 : R-values as a function of image number (measurements)

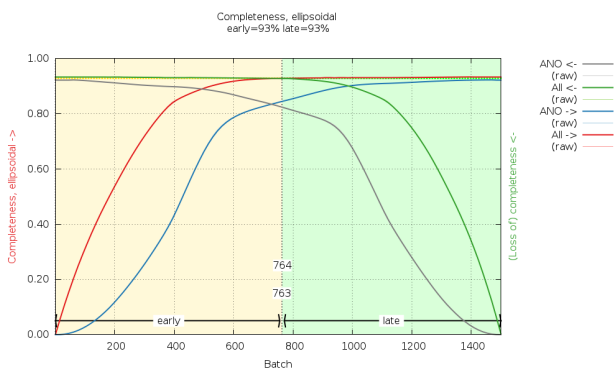


Fig.20 : Completeness (ellipsoidal) as a function of image number (measurements)

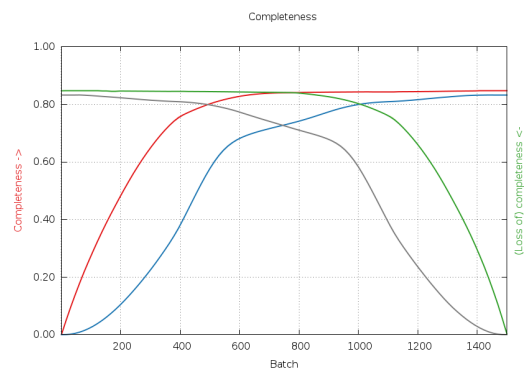


Fig.21 : Completeness (spherical) as a function of image number (measurements)

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

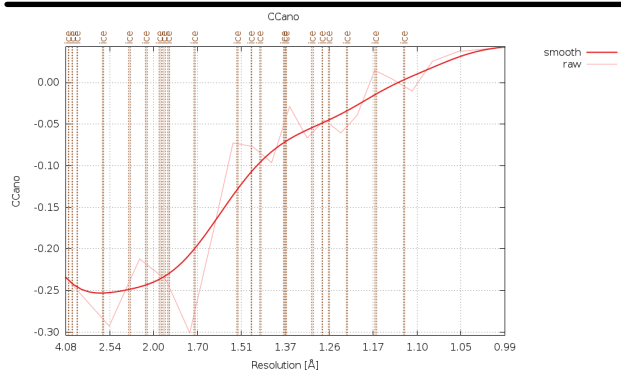


Fig.22 : CCano as a function of resolution (measurements)

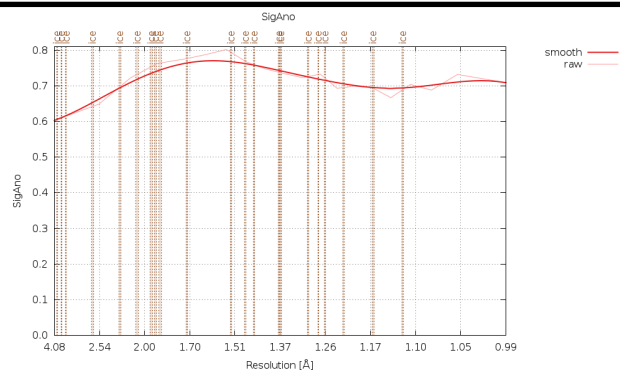


Fig.23 : SigAno as a function of resolution (measurements)

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. *Acta Cryst.* D67, 293-302.
- XDS Kabsch, W. (2010). XDS. *Acta Cryst.* D66, 125-132.
- 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.