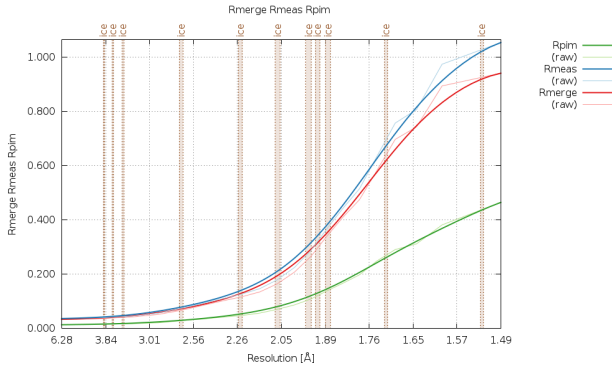| autoPROC	1.1.7 (20200319)
XDS	VERSION Jan 31, 2020 BUILT=20200131
AIMLESS	Version 0.7.4
STARANISO	Version 2.3.28 (1-Mar-2020)
CCP4	Version 7.0.078
Host	server8
User	vonrhein (group = users)
Date	Thu Mar 19 13:30:31 CET 2020
autoPROC	/home/software/xtal/GPhL/20200319
	P1P7_G4_X1_#####.cbf (1199 images, 179.85°)

Anisotropic data analysis with STARANISO:

Spacegroup	P212121
Cell parameters	80.907 88.869 128.704
	90.0 90.0 90.0
Wavelength [A]	0.97926
Diffraction limits [A]	1.809 1.550 1.423
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_*
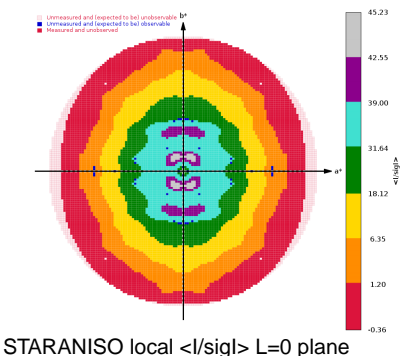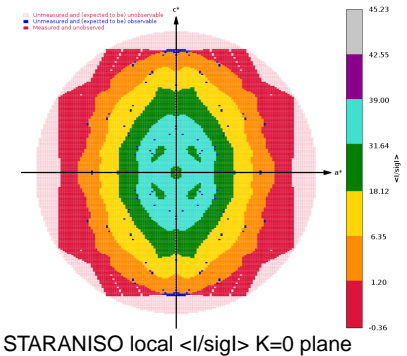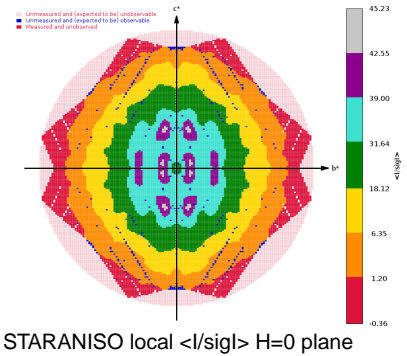
	Overall	Inner Shell	Outer Shell
Low resolution limit	73.130	73.130	1.568
High resolution limit	1.423	4.446	1.423
Rmerge (all I+ & I-)	0.068	0.034	0.941
Rmeas (all I+ & I-)	0.073	0.037	1.054
Rpim (all I+ & I-)	0.029	0.014	0.465
Total number of observations	786910	37566	29759
Total number unique	121041	6051	6053
Mean(I)/sd(I)	13.2	37.4	1.5
Completeness (spherical)	69.7	99.8	13.9
Completeness (ellipsoidal)	95.4	99.8	71.3
Multiplicity	6.5	6.2	4.9
CC(1/2)	0.999	0.999	0.731
Anomalous completeness (spherical)	68.8	99.8	13.3
Anomalous completeness (ellipsoidal)	95.1	99.8	70.3
Anomalous multiplicity	3.4	3.4	2.6
CC(ano)	-0.119	-0.178	-0.013
|DANO|/sd(DANO)	0.713	0.714	0.691

STARANISO local <I/sigI> H=0 plane

STARANISO local <I/sigI> K=0 plane
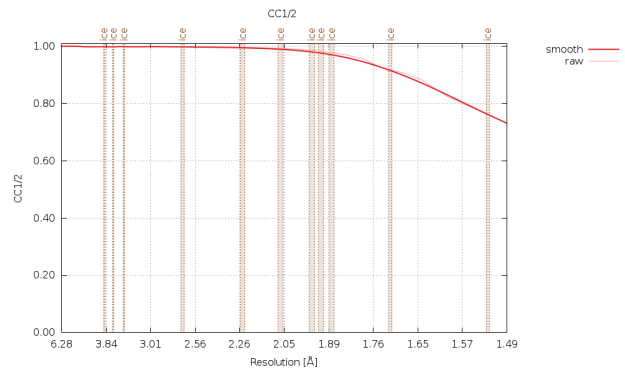

STARANISO local <I/sigI> L=0 plane

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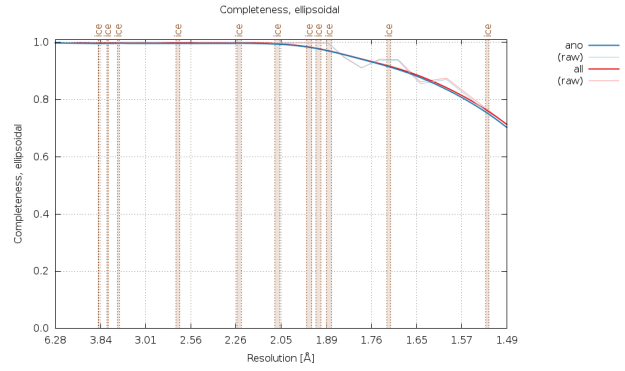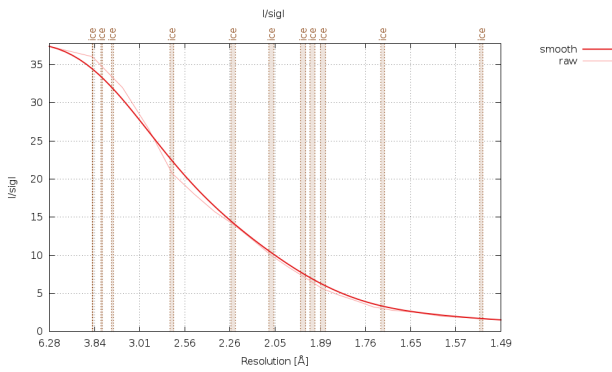

Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.
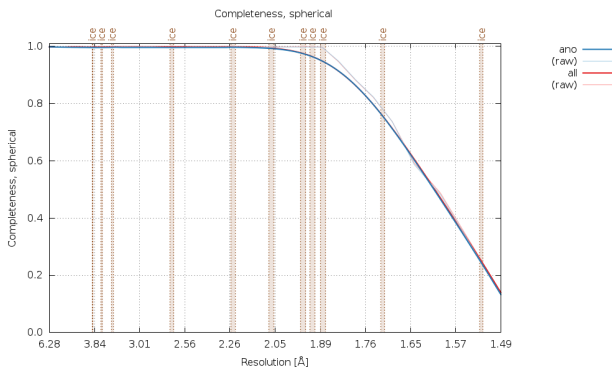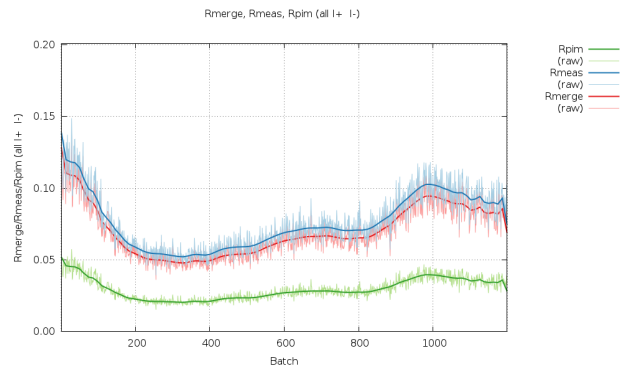

Fig.3 : Completeness (spherical) as a function of resolution (observations)
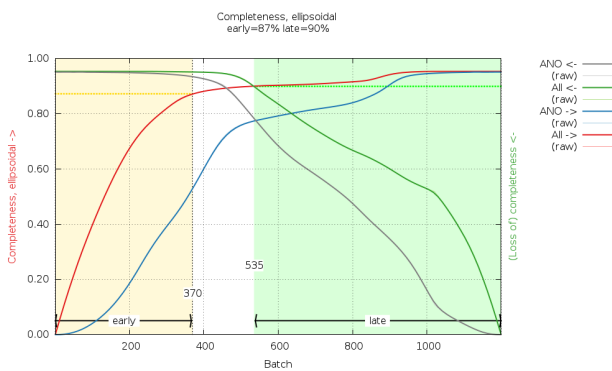

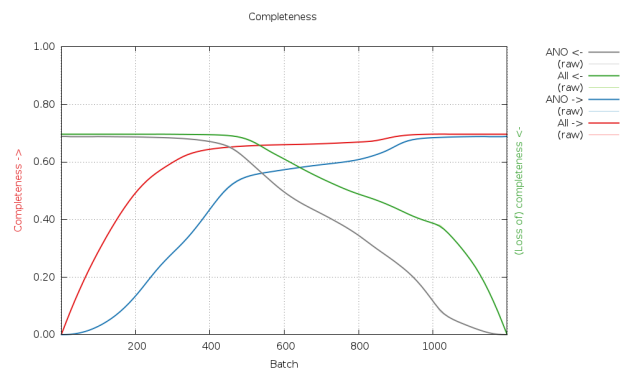**Fig.4 :** CC1/2 as a function of resolution (observations)

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

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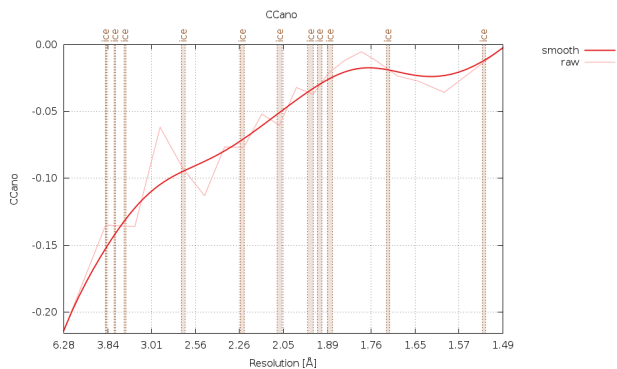

Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.
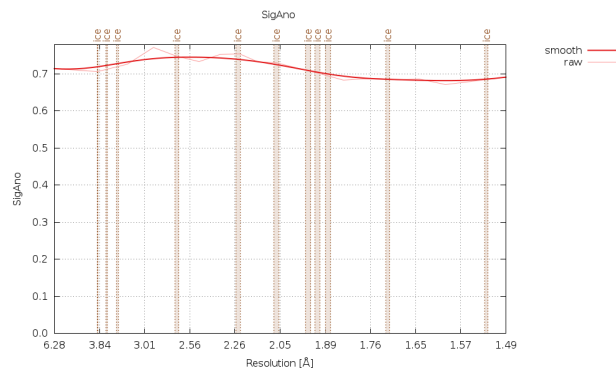

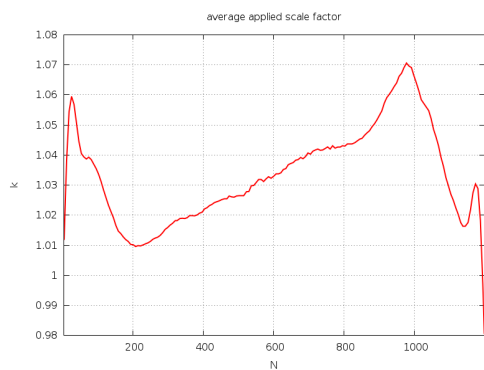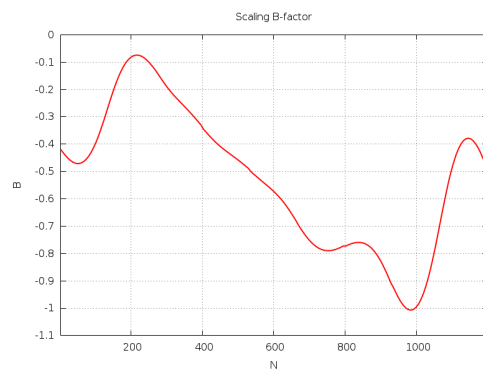**Fig.8 :** Completeness (spherical) as a function of image number (observations)

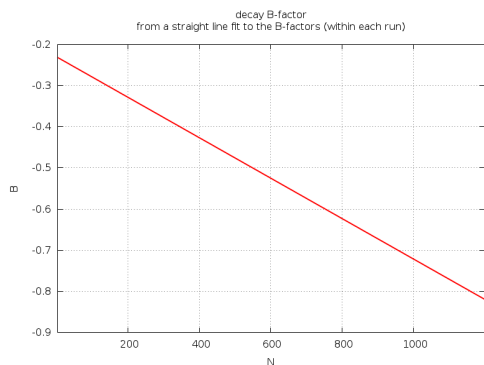**Fig.9 :** CCano as a function of resolution (observations)

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

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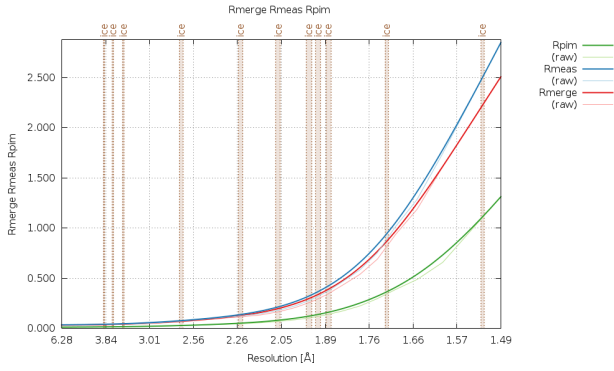

Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)
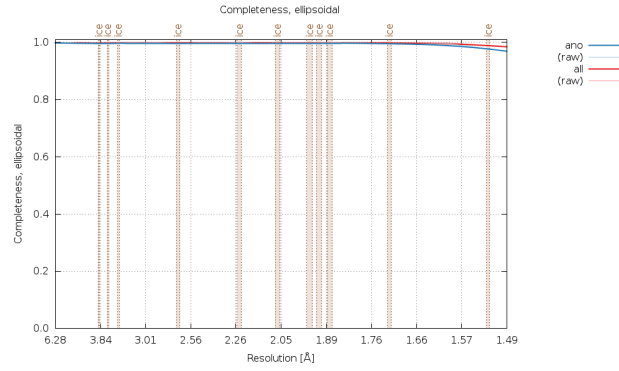

Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)
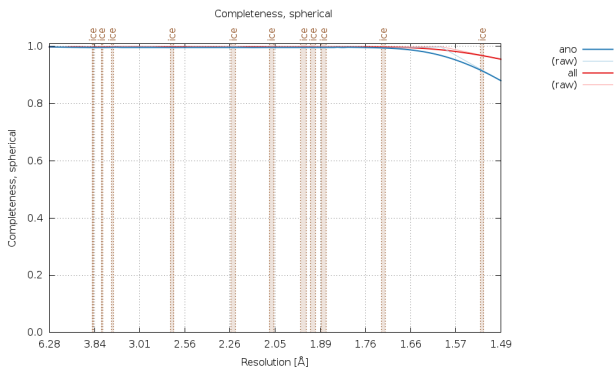
Fig.14 : R-values as a function of resolution (measurements)

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)
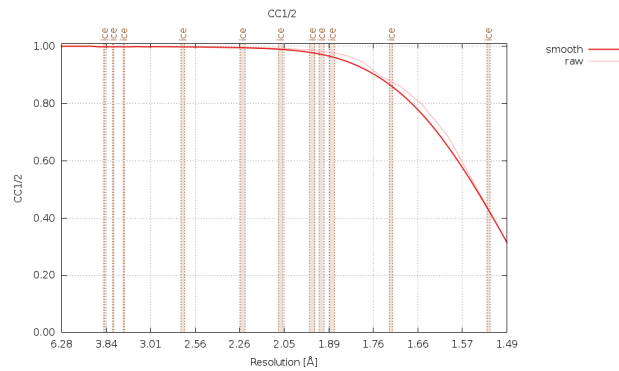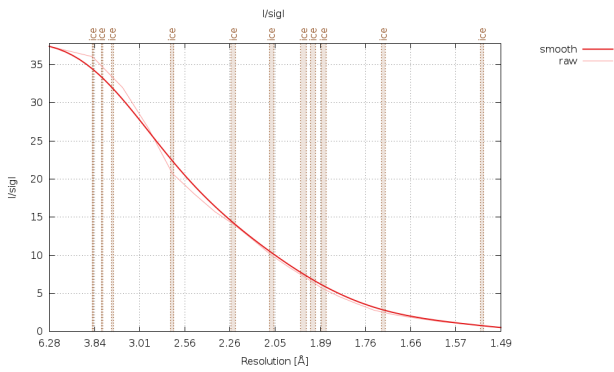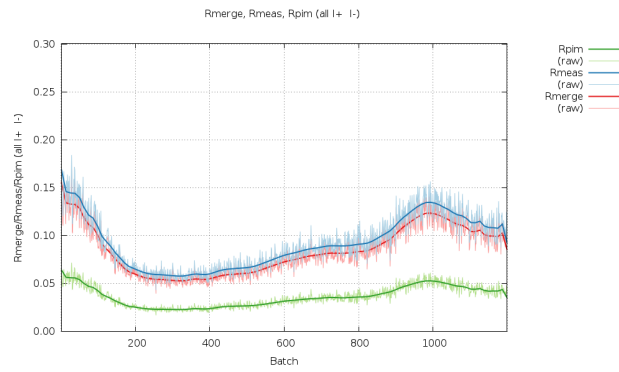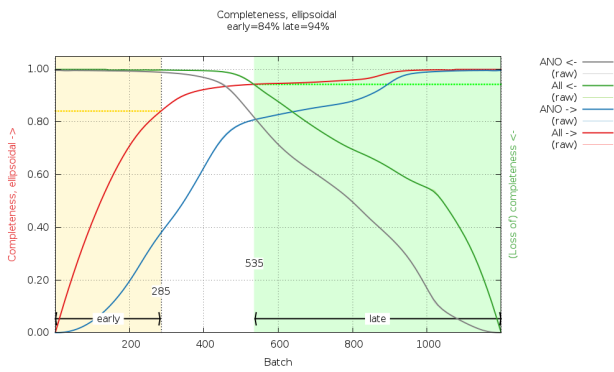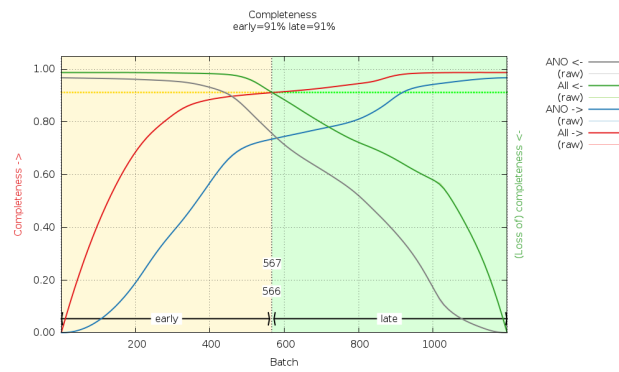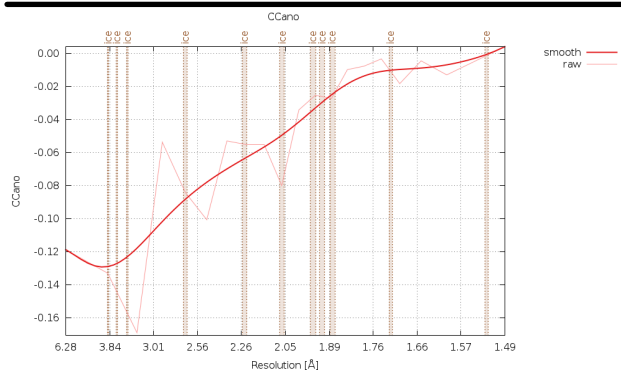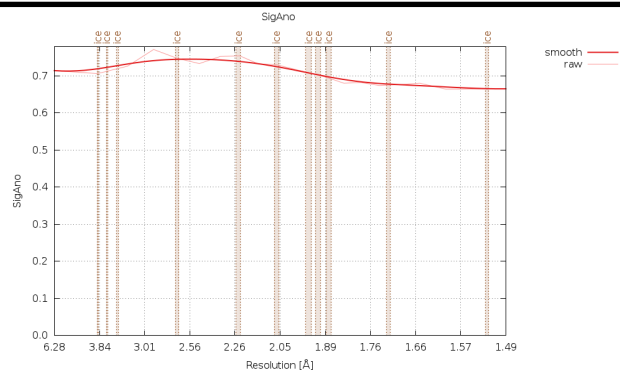

Fig.22 : CCano as a function of resolution (measurements)

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

References

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POINTLESS	Evans, P.R. (2006). Scaling and assessment of data quality, Acta Cryst. D62, 72-82.
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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.
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