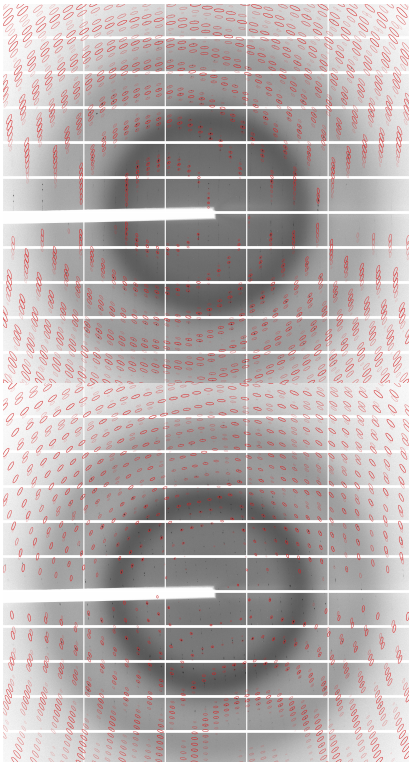

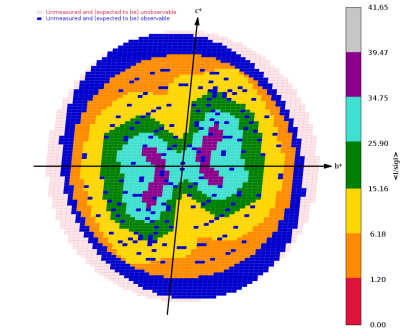

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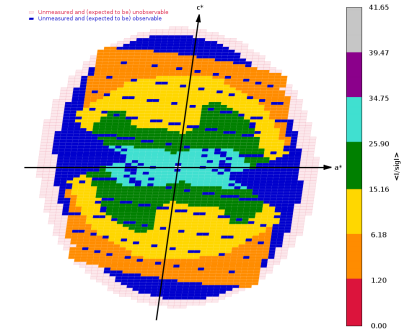

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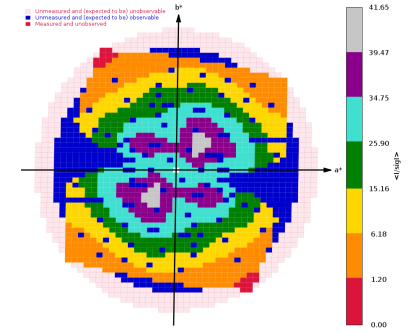

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AIMLESS	Version 0.7.4
STARANISO	Version 2.3.33 (11-Apr-2020)
CCP4	Version 7.0.078
Host	server8
User	vonrhein (group = users)
Date	Tue Apr 21 22:11:07 CEST 2020
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2a	m1a2peg-2_#####.cbf (300 images, 150°)
3a	m1a2peg-3_#####.cbf (350 images, 175°)

Anisotropic data analysis with STARANISO:

Spacegroup	P1
Cell parameters	30.1468 37.7807 64.8130
	95.8014 97.9852 90.1138
Wavelength [A]	0.97918
Diffraction limits [A]	1.517 1.561 1.361
Eigenvector-1	0.942 -0.274 0.196
Eigenvector-2	0.141 0.849 0.509
Eigenvector-3	-0.306 -0.452 0.838
Direction-1	0.922 _a_* - 0.338 _b_* + 0.190 _c_*
Direction-2	0.103 _a_* + 0.776 _b_* + 0.622 _c_*
Direction-3	-0.148 _a_* - 0.274 _b_* + 0.950 _c_*

	Overall	Inner Shell	Outer Shell
Low resolution limit	37.582	37.582	1.485
High resolution limit	1.361	3.749	1.361
Rmerge (all I+ & I-)	0.115	0.053	1.297
Rmeas (all I+ & I-)	0.142	0.067	1.553
Rpim (all I+ & I-)	0.082	0.040	0.845
Total number of observations	111570	6592	5173
Total number unique	37349	2535	1643
Mean(I)/sd(I)	12.5	31.8	1.4
Completeness (spherical)	61.8	88.6	11.9
Completeness (ellipsoidal)	75.2	88.6	14.2
Multiplicity	3.0	2.6	3.1
CC(1/2)	0.990	0.987	0.138
Anomalous completeness (spherical)	54.4	77.3	10.0
Anomalous completeness (ellipsoidal)	66.3	77.3	12.1
Anomalous multiplicity	1.6	1.4	1.7
CC(ano)	-0.169	-0.185	0.038
|DANO|/sd(DANO)	0.988	0.950	1.062

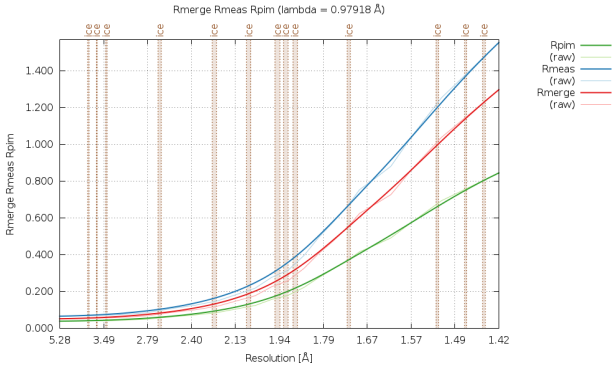

Fig.1 : R-values as a function of resolution (observations)

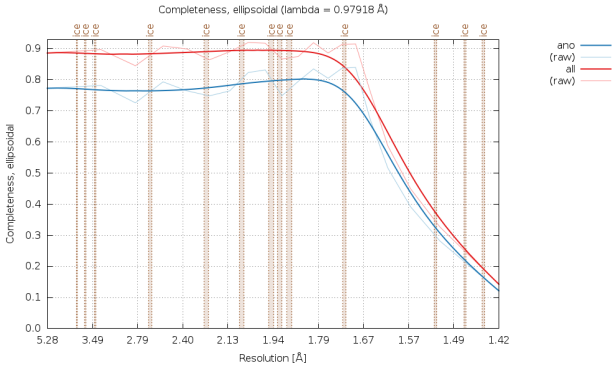

Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.

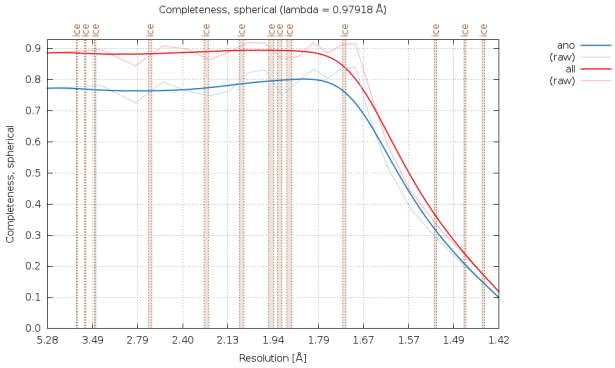

Fig.3 : Completeness (spherical) as a function of resolution (observations)

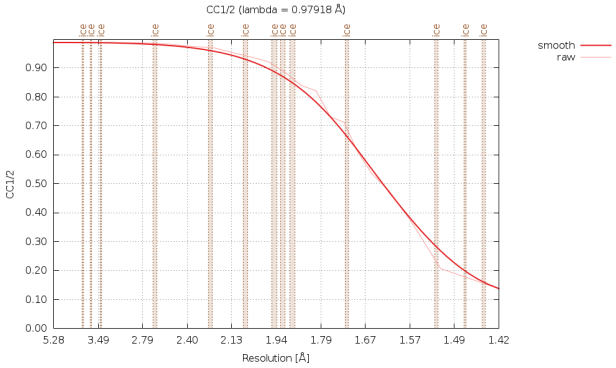

Fig.4 : CC1/2 as a function of resolution (observations)

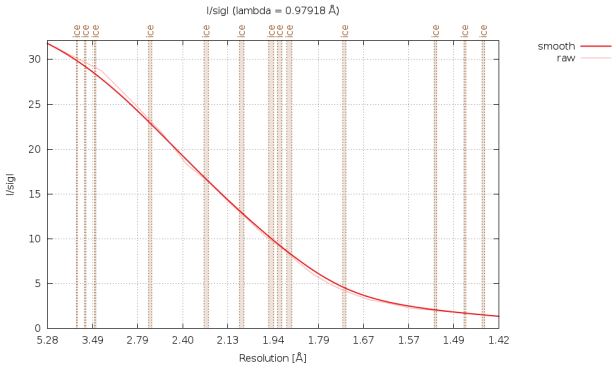

Fig.5 : I/sigI as a function of resolution (observations)

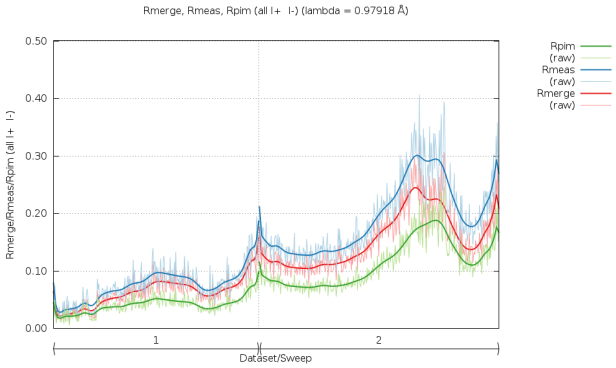

Fig.6 : R-values as a function of image number (observations)

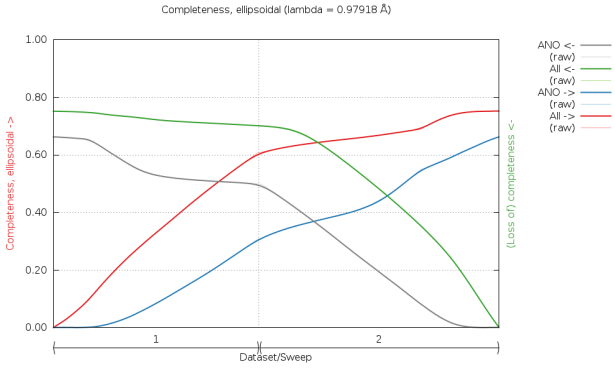

Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.

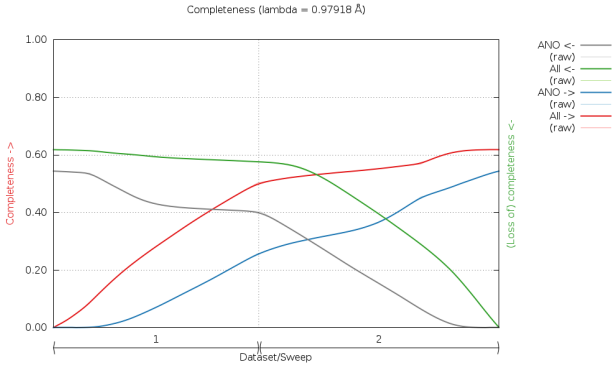

Fig.8 : Completeness (spherical) as a function of image number (observations)

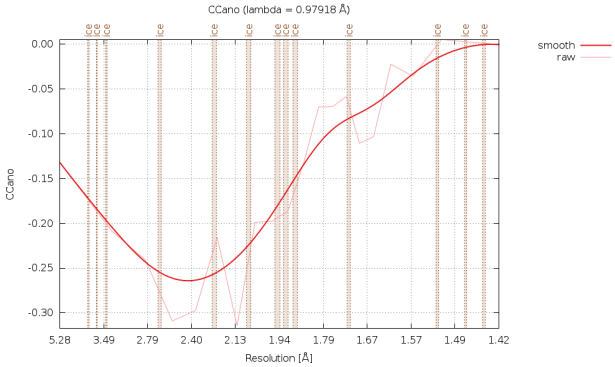

Fig.9 : CCano as a function of resolution (observations)

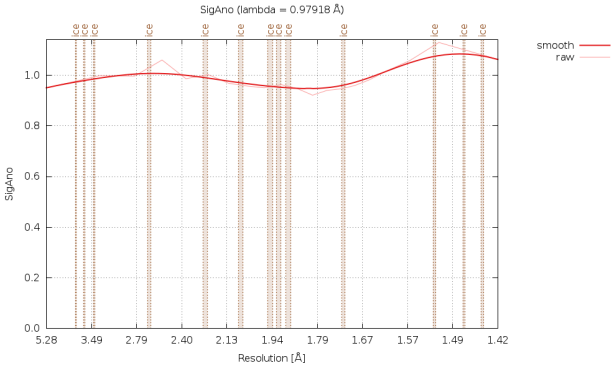

Fig.10 : SigAno as a function of resolution (observations)

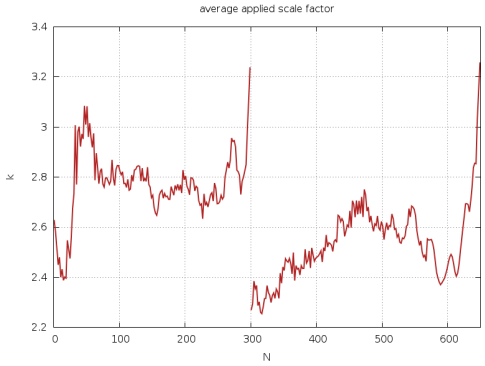

Fig.11 : Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

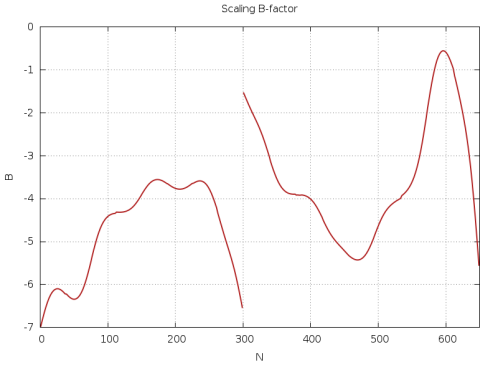

Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

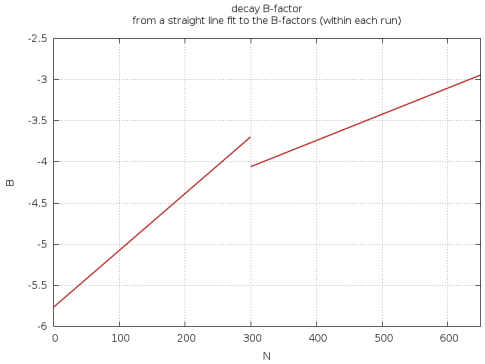

Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

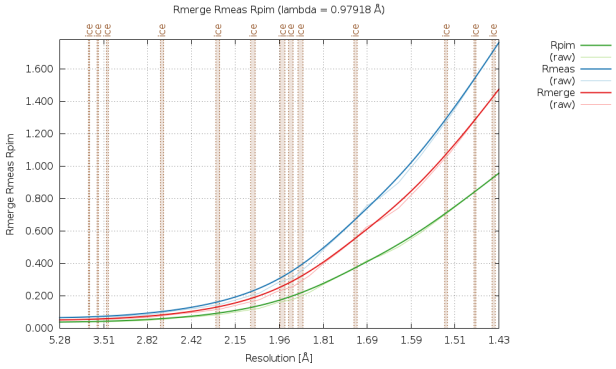

Fig.14 : R-values as a function of resolution (measurements)

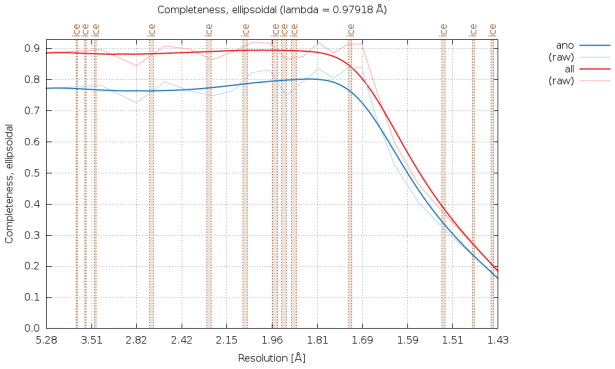

Fig.15 : Completeness (ellipsoidal) as a function of resolution (measurements)

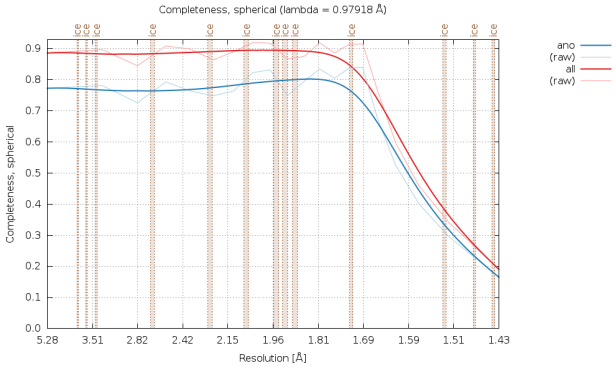

Fig.16 : Completeness (spherical) as a function of resolution (measurements)

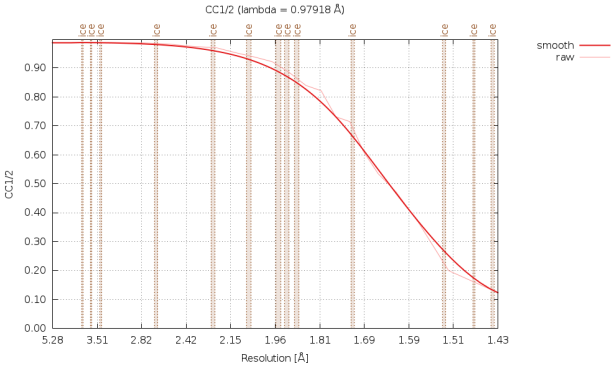

Fig.17 : CC1/2 as a function of resolution (measurements)

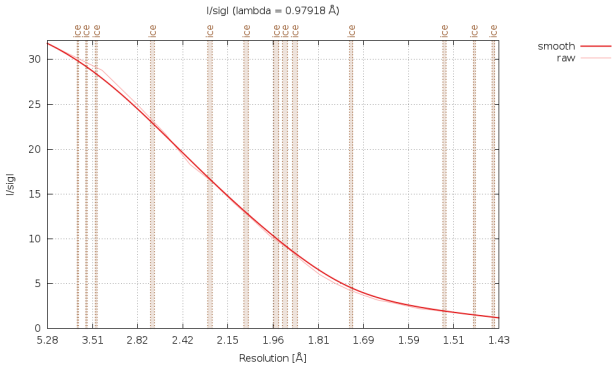

Fig.18 : I/sigI as a function of resolution (measurements)

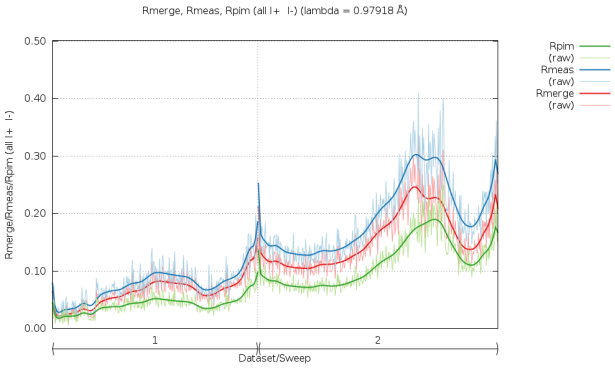

Fig.19 : R-values as a function of image number (measurements)

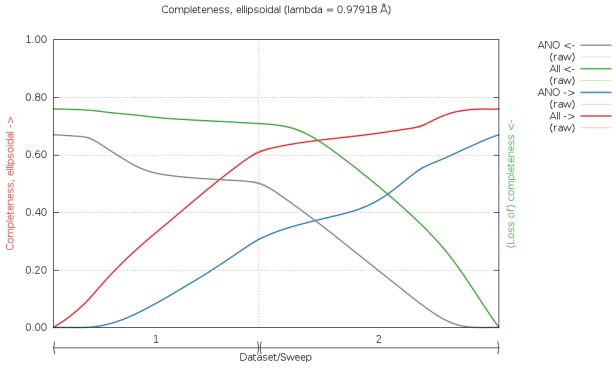

Fig.20 : Completeness (ellipsoidal) as a function of image number (measurements)

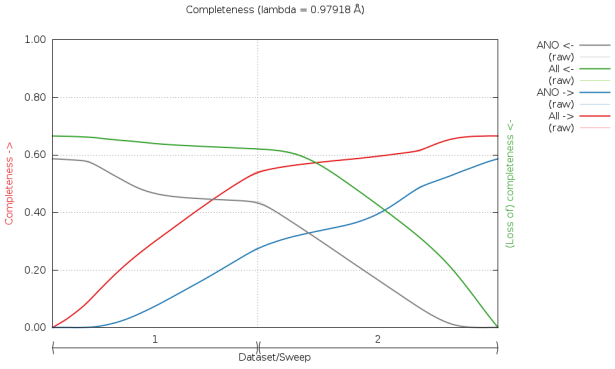

Fig.21 : Completeness (spherical) as a function of image number (measurements)

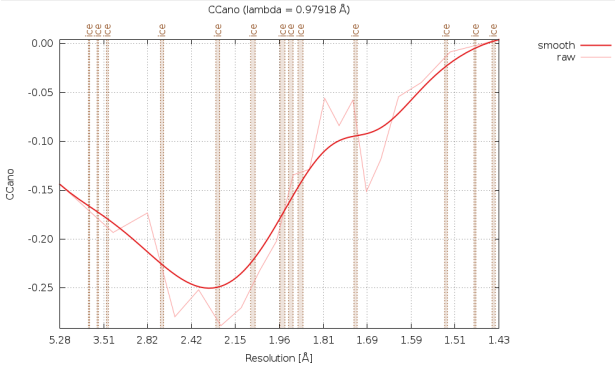

Fig.22 : CCano as a function of resolution (measurements)

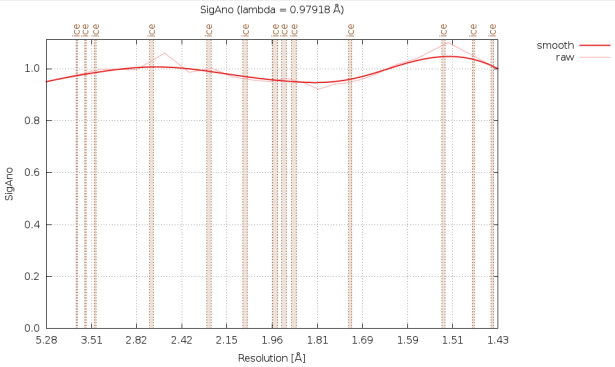

Fig.23 : SigAno as a function of resolution (measurements)

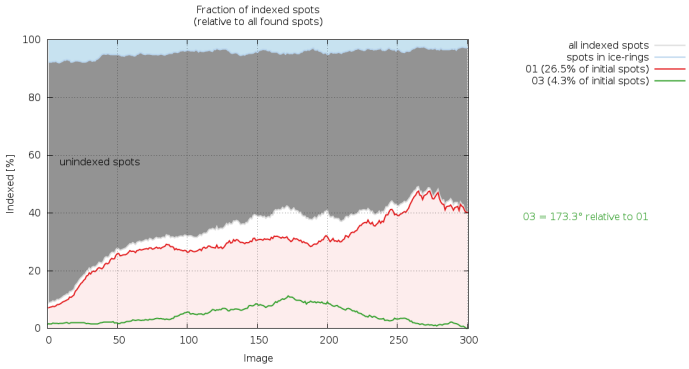

Fig.24 : (sweep 2a) number of spots for each indexing solution as a function of image number

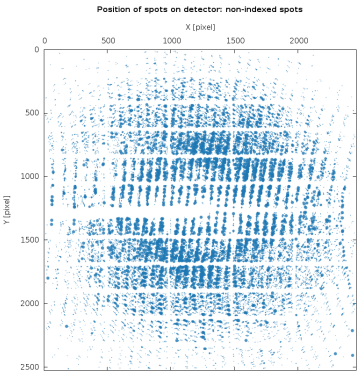

Fig.25 : (sweep 2a) unindexed spots as a function of detector position

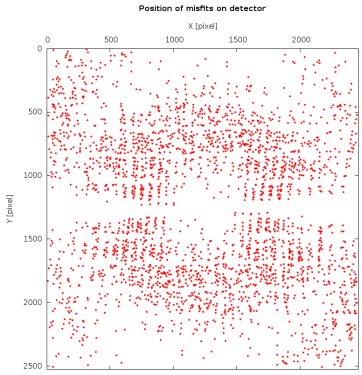

Fig.26 : (sweep 2a) reflections classified as misfits (as a function of detector position)

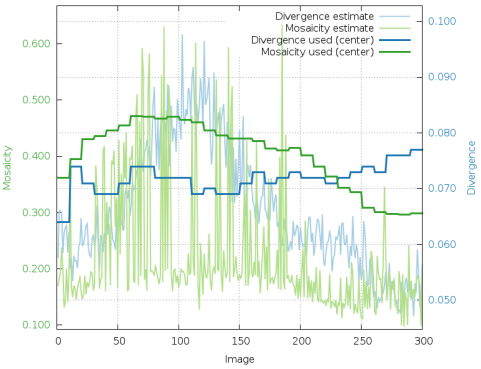

Fig.27 : (sweep 2a) divergence and mosaicity (estimated and used) as a function of image number

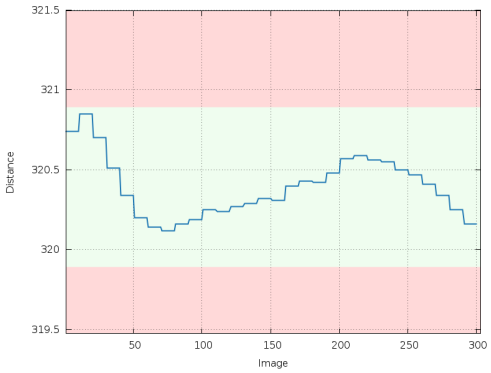

Fig.28 : (sweep 2a) refined crystal-to-detector distance as a function of image number

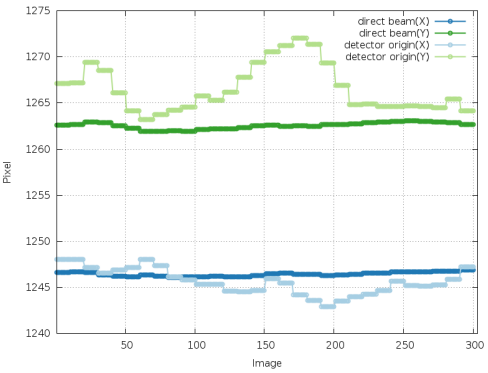

Fig.29 : (sweep 2a) direct beam position and detector origin as a function of image number

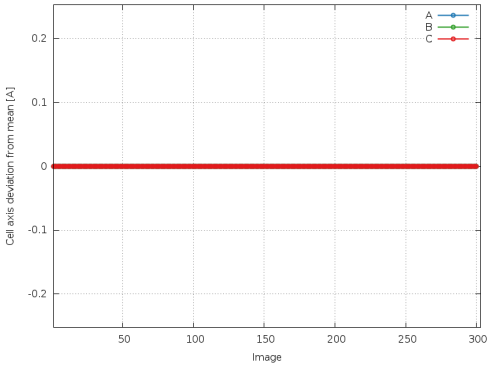

Fig.30 : (sweep 2a) deviation of refined cell axes relative to their mean (as a function of image number)

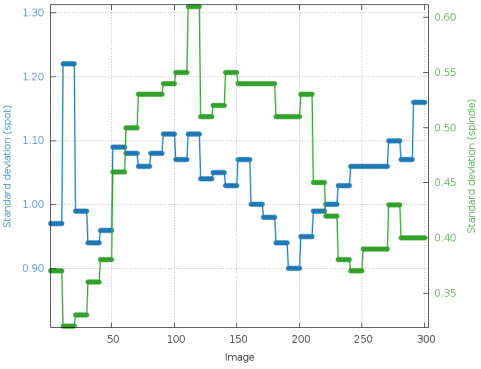

Fig.31 : (sweep 2a) standard deviation (spot position and spindle) as a function of image number

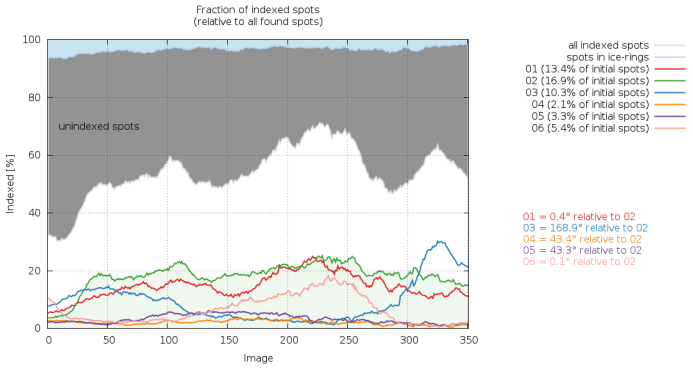

Fig.32 : (sweep 3a) number of spots for each indexing solution as a function of image number

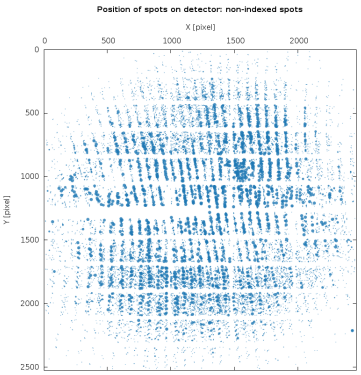

Fig.33 : (sweep 3a) unindexed spots as a function of detector position

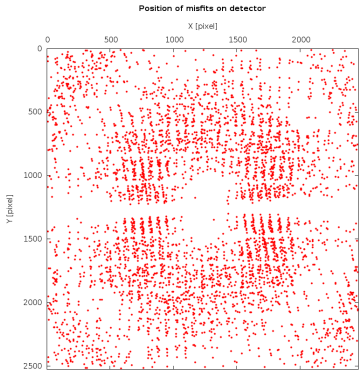

Fig.34 : (sweep 3a) reflections classified as misfits (as a function of detector position)

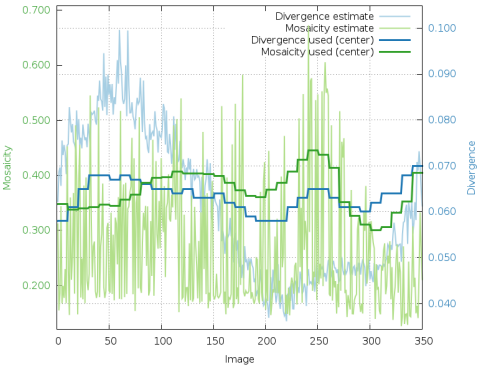

Fig.35 : (sweep 3a) divergence and mosaicity (estimated and used) as a function of image number

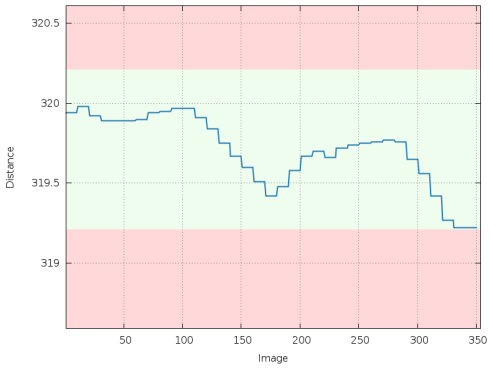

Fig.36 : (sweep 3a) refined crystal-to-detector distance as a function of image number

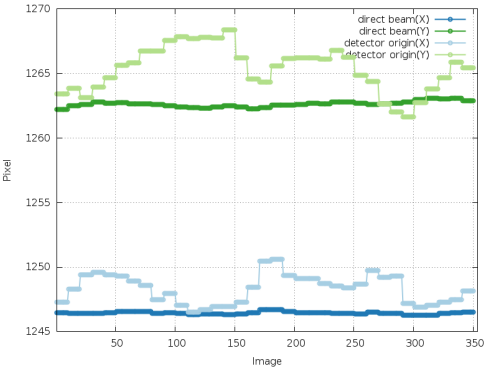

Fig.37 : (sweep 3a) direct beam position and detector origin as a function of image number

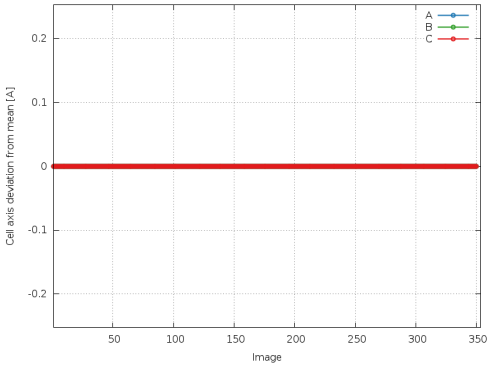

Fig.38 : (sweep 3a) deviation of refined cell axes relative to their mean (as a function of image number)

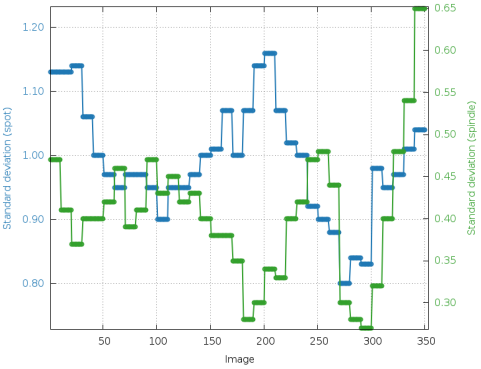

Fig.39 : (sweep 3a) standard deviation (spot position and spindle) as a function of image number

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.