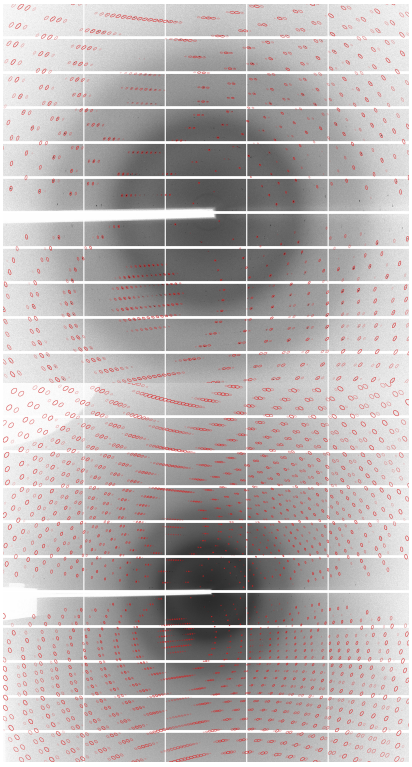

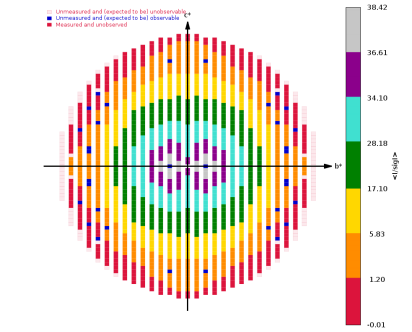

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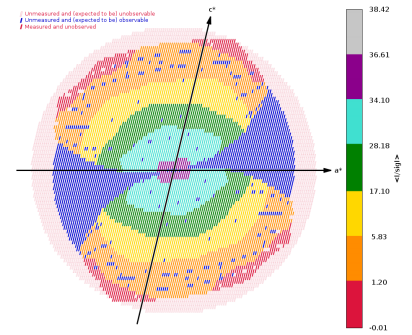

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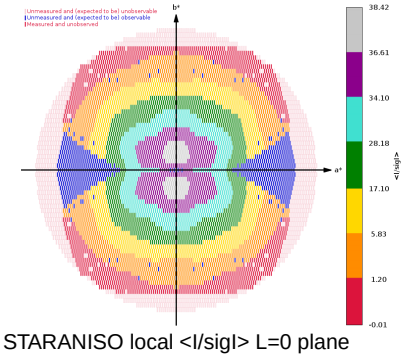

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XDS	VERSION Jan 31, 2020 BUILT=20200131
AIMLESS	Version 0.7.4
STARANISO	Version 2.3.33 (11-Apr-2020)
CCP4	Version 7.0.078
Host	server8
User	vonrhein (group = users)
Date	Fri Apr 24 08:42:24 CEST 2020
autoPROC	/home/software/xtal/GPhL/20200420
ADRP_Pmin_F11_d1_data	ADRP_Pmin_F11_d1_data_#####.cbf (720 images, 360°)
ADRP_Pmin_F11_d1_data2	ADRP_Pmin_F11_d1_data2_#####.cbf (200 images, 100°)

Anisotropic data analysis with STARANISO:

Spacegroup	C2
Cell parameters	139.5938 29.6609 37.8595 90.0000 103.5076 90.0000
Wavelength [A]	0.97918
Diffraction limits [A]	1.137 1.169 1.081
Eigenvector-1	0.929 0.000 -0.371
Eigenvector-2	0.000 1.000 0.000
Eigenvector-3	0.371 0.000 0.929
Direction-1	0.986 _a_* - 0.166 _c_*
Direction-2	_b_*
Direction-3	0.858 _a_* + 0.513 _c_*

	Overall	Inner Shell	Outer Shell
Low resolution limit	36.083	36.083	1.169
High resolution limit	1.081	3.149	1.081
Rmerge (all I+ & I-)	0.118	0.056	0.581
Rmeas (all I+ & I-)	0.129	0.060	0.743
Rpim (all I+ & I-)	0.049	0.021	0.459
Total number of observations	264271	21814	4685
Total number unique	47849	2712	2279
Mean(I)/sd(I)	12.0	34.2	1.5
Completeness (spherical)	73.8	98.4	16.9
Completeness (ellipsoidal)	82.9	98.4	32.4
Multiplicity	5.5	8.0	2.1
CC(1/2)	0.995	0.998	0.437
Anomalous completeness (spherical)	56.6	99.3	8.8
Anomalous completeness (ellipsoidal)	64.1	99.3	18.0
Anomalous multiplicity	3.4	4.3	1.3
CC(ano)	-0.100	-0.158	NA
|DANO|/sd(DANO)	0.731	0.687	0.637

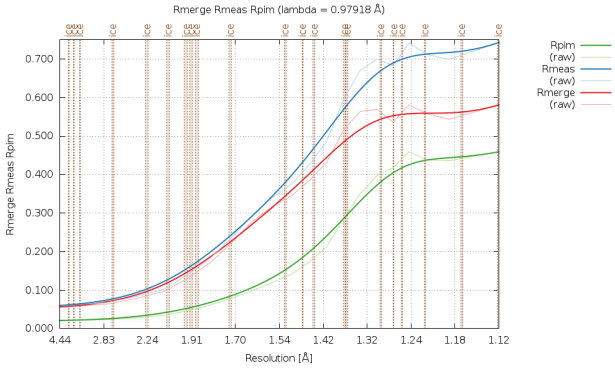

Fig.1 : R-values as a function of resolution (observations)

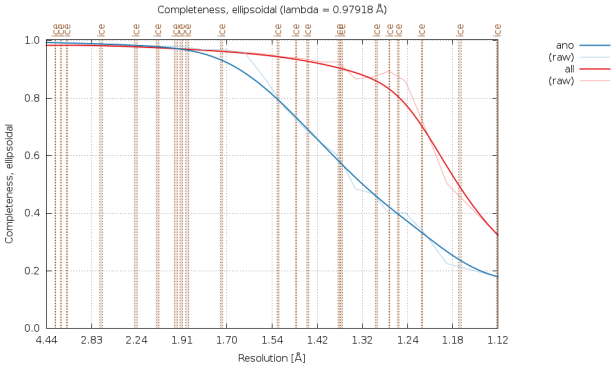

Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.

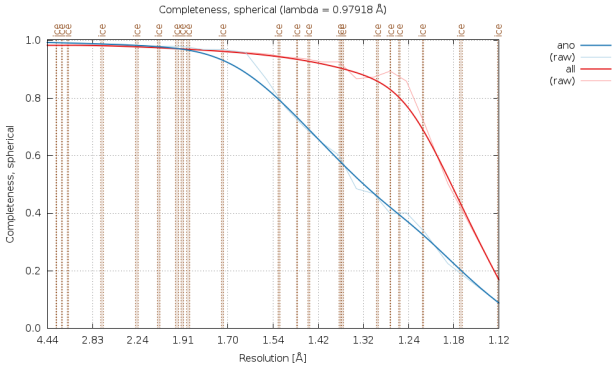

Fig.3 : Completeness (spherical) as a function of resolution (observations)

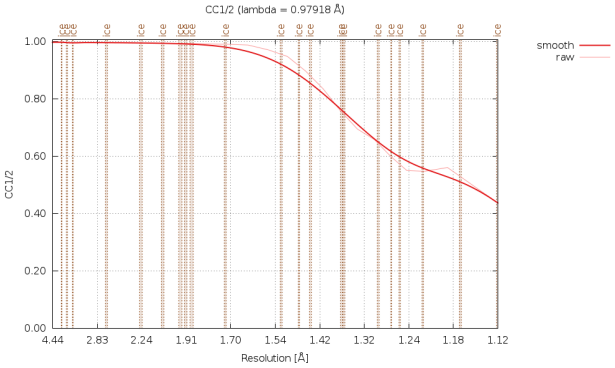

Fig.4 : CC1/2 as a function of resolution (observations)

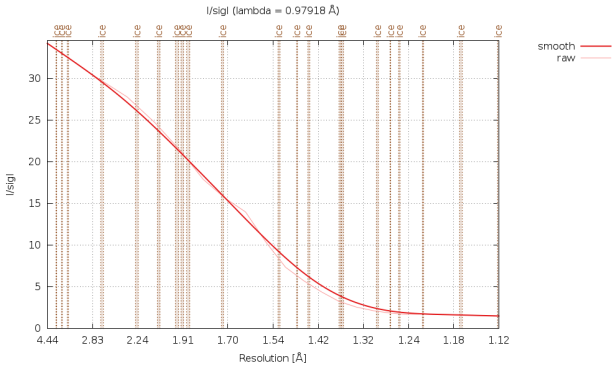

Fig.5 : I/sigI as a function of resolution (observations)

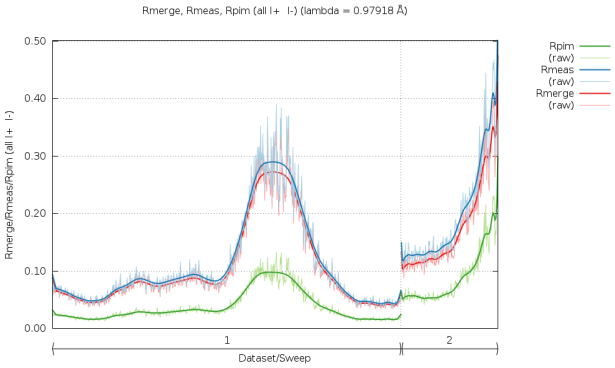

Fig.6 : R-values as a function of image number (observations)

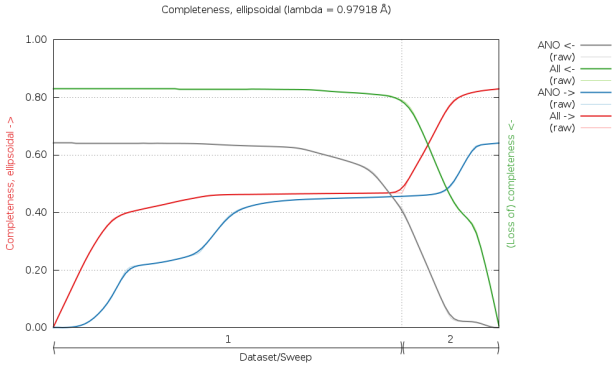

Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.

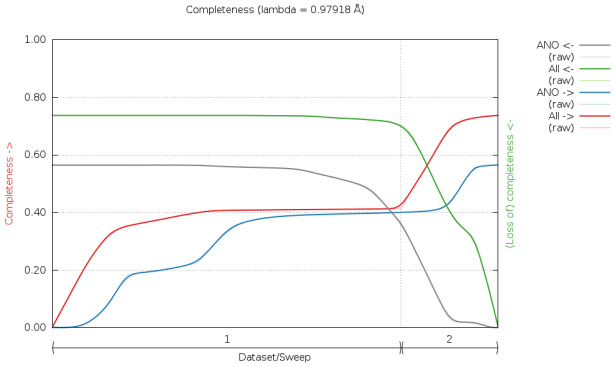

Fig.8 : Completeness (spherical) as a function of image number (observations)

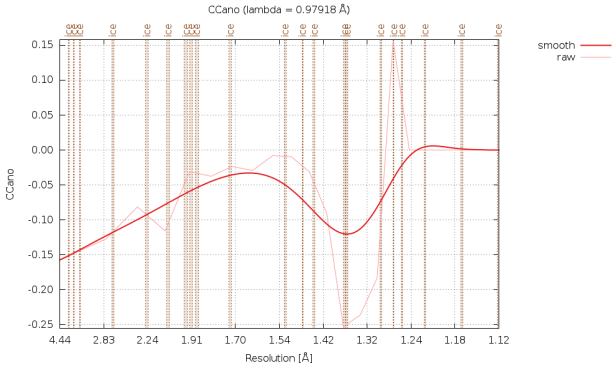

Fig.9 : CCano as a function of resolution (observations)

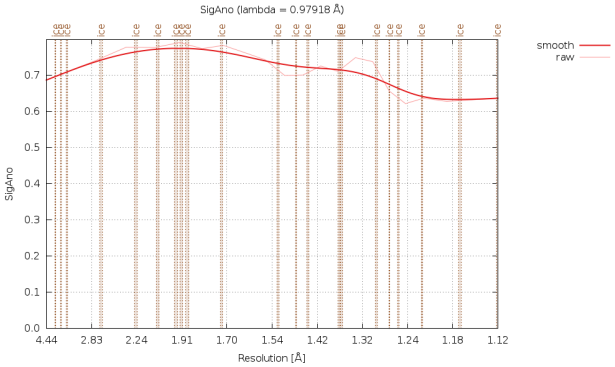

Fig.10 : SigAno as a function of resolution (observations)

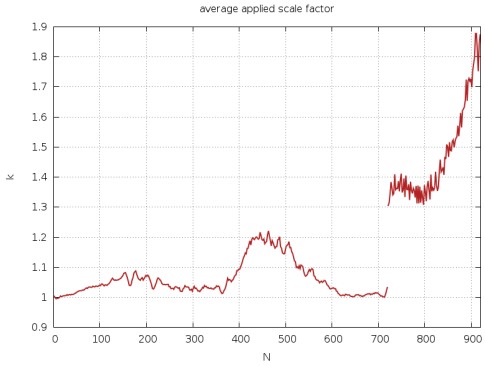

Fig.11 : Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

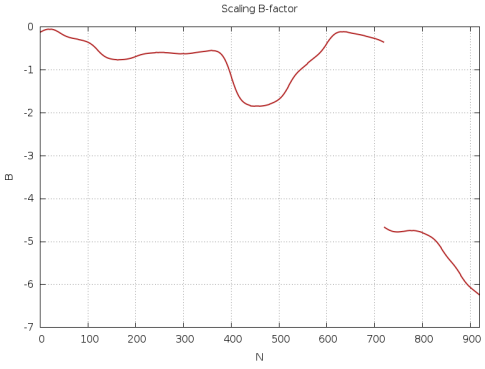

Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

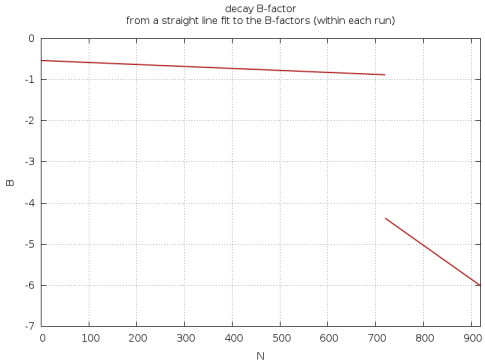

Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

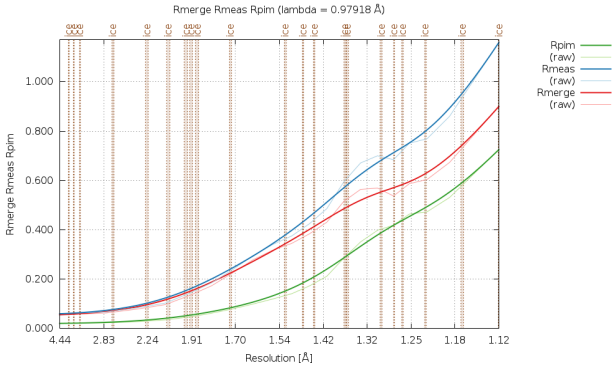

Fig.14 : R-values as a function of resolution (measurements)

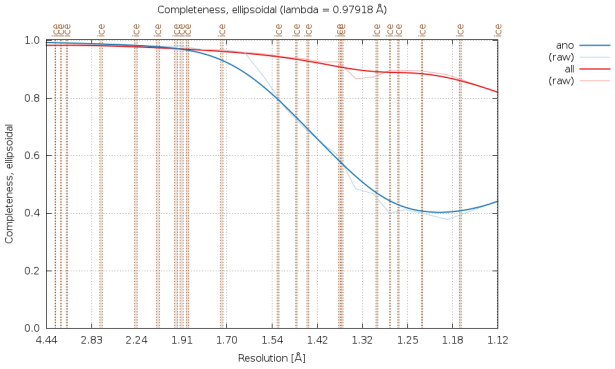

Fig.15 : Completeness (ellipsoidal) as a function of resolution (measurements)

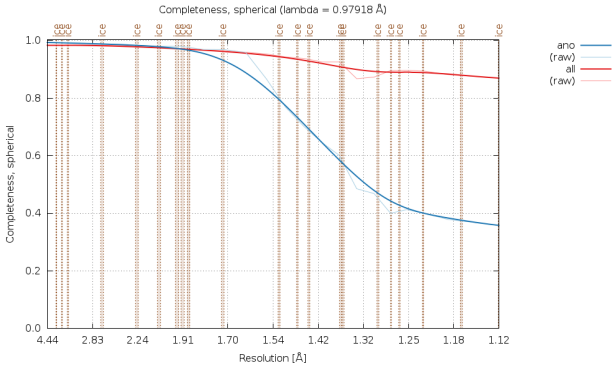

Fig.16 : Completeness (spherical) as a function of resolution (measurements)

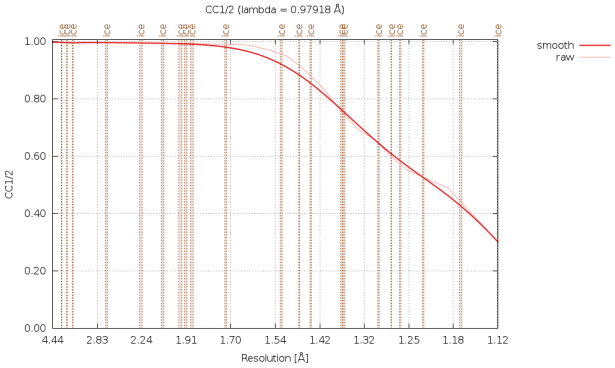

Fig.17 : CC1/2 as a function of resolution (measurements)

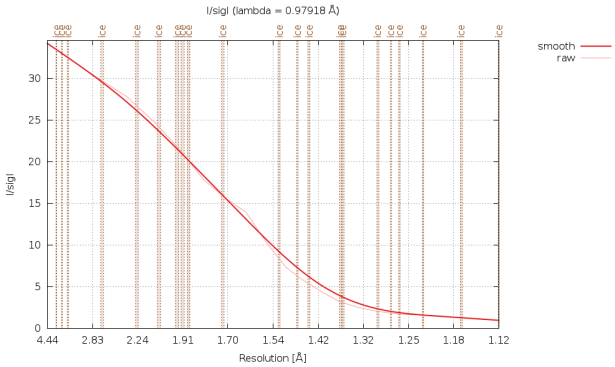

Fig.18 : I/sigI as a function of resolution (measurements)

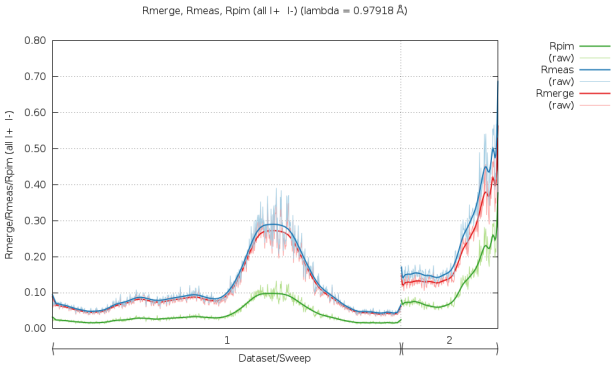

Fig.19 : R-values as a function of image number (measurements)

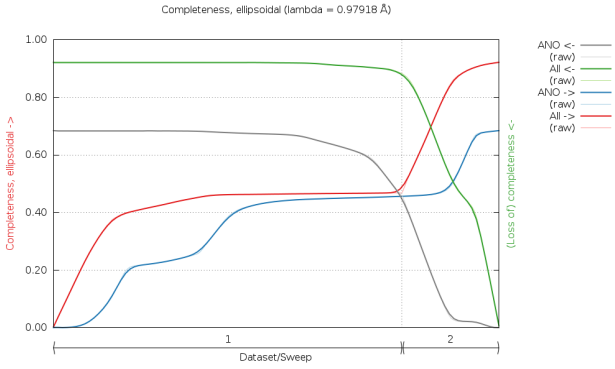

Fig.20 : Completeness (ellipsoidal) as a function of image number (measurements)

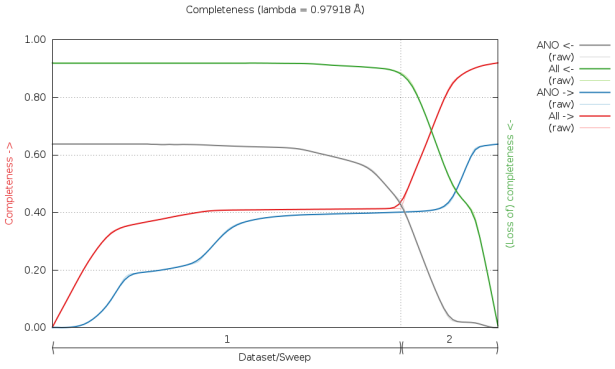

Fig.21 : Completeness (spherical) as a function of image number (measurements)

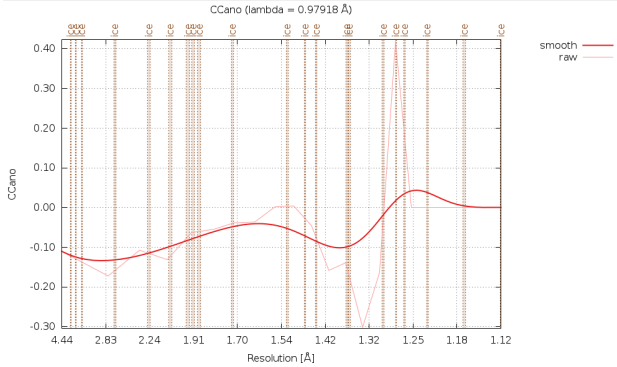

Fig.22 : CCano as a function of resolution (measurements)

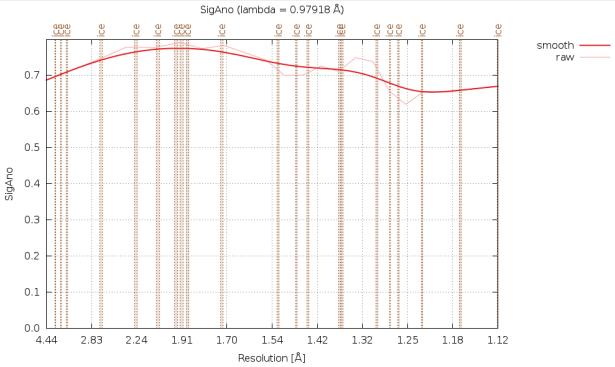

Fig.23 : SigAno as a function of resolution (measurements)

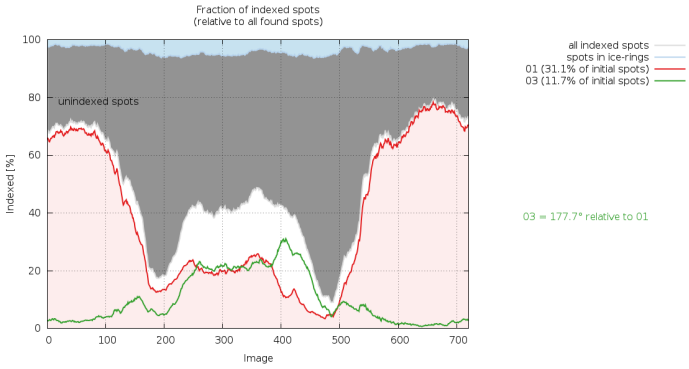

Fig.24 : (sweep ADRP_Pmin_F11_d1_data) number of spots for each indexing solution as a function of image number

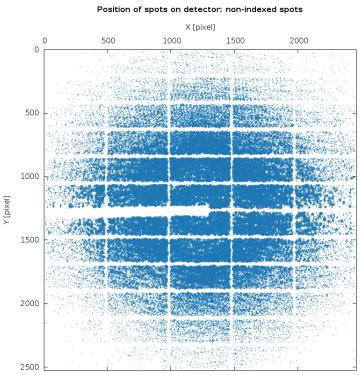

Fig.25 : (sweep ADRP_Pmin_F11_d1_data) unindexed spots as a function of detector position

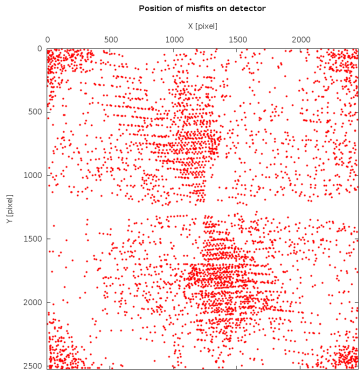

Fig.26 : (sweep ADRP_Pmin_F11_d1_data) reflections classified as misfits (as a function of detector position)

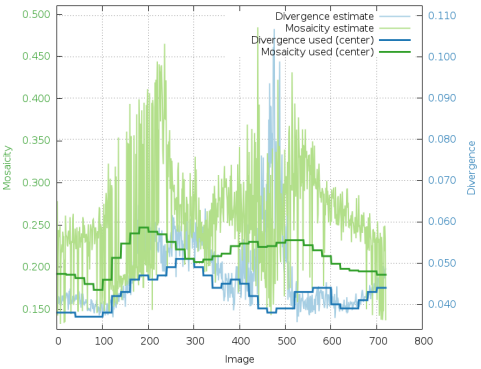

Fig.27 : (sweep ADRP_Pmin_F11_d1_data) divergence and mosaicity (estimated and used) as a function of image number

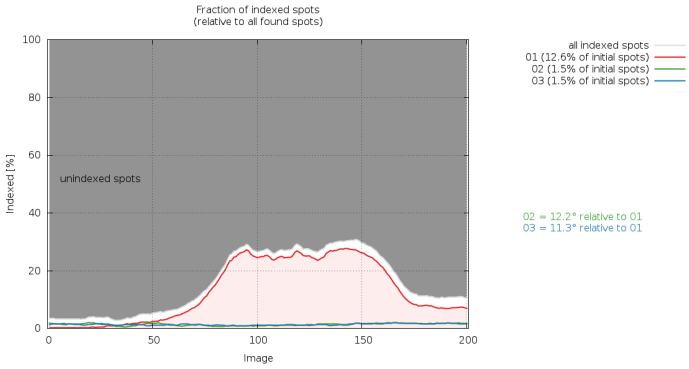

Fig.28 : (sweep ADRP_Pmin_F11_d1_data2) number of spots for each indexing solution as a function of image number

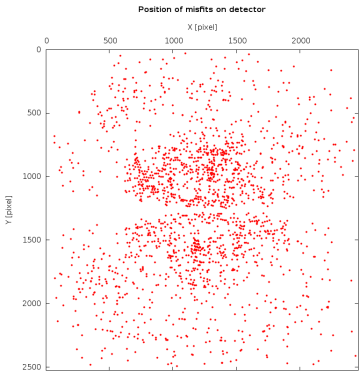

Fig.29 : (sweep ADRP_Pmin_F11_d1_data2) reflections classified as misfits (as a function of detector position)

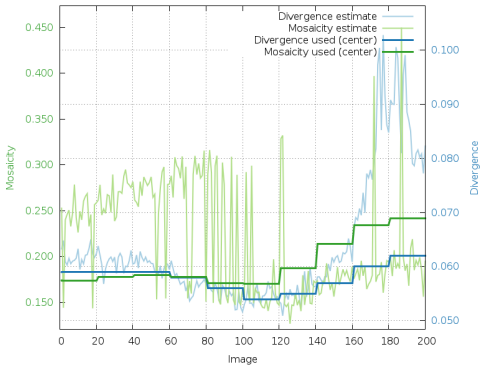

Fig.30 : (sweep ADRP_Pmin_F11_d1_data2) divergence and mosaicity (estimated and used) as a function of image number

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.