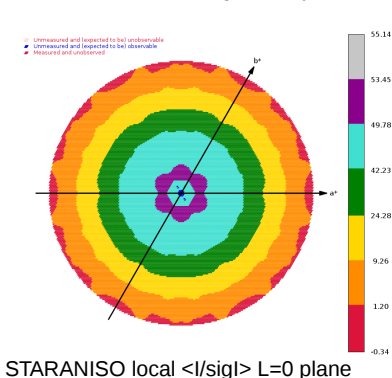
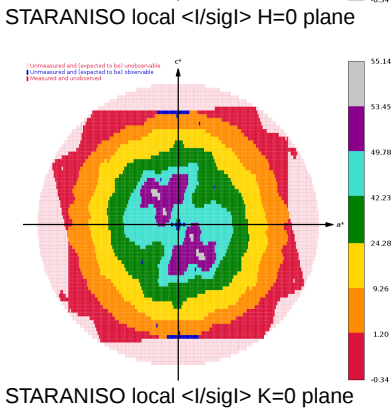
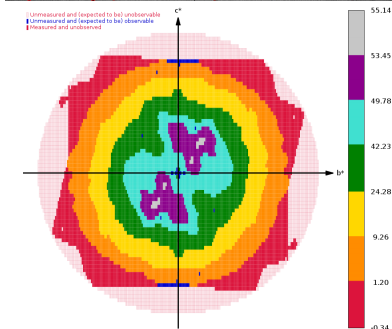
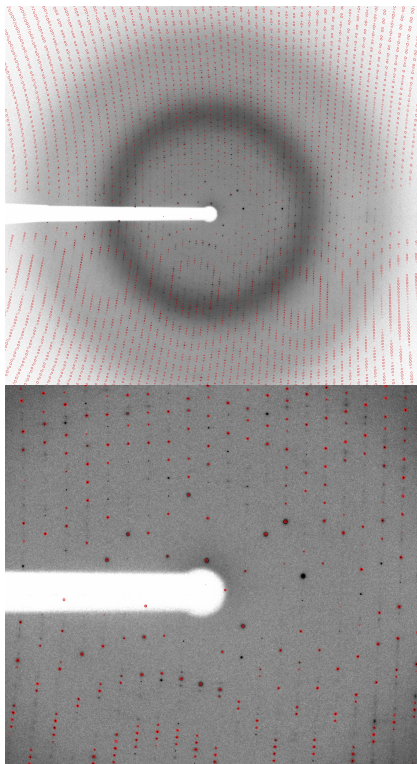




autoPROC 1.3.0 (20200318)
XDS VERSION Jan 31, 2020 BUILT=20200131
AIMLESS Version 0.7.4
STARANISO Version 2.3.33 (11-Apr-2020)
CCP4 Version 7.0.078
Host server8
User vonrhein (group = users)
Date Mon Apr 20 11:34:38 CEST 2020
autoPROC /home/software/xtal/GPhL/20200420
idp51000-201-a_1_2_3.### (195 images, 117°)

Anisotropic data analysis with STARANISO:

Spacegroup P3121
Cell parameters 167.722 167.722 51.941
90.0 90.0 120.0
Wavelength [Å] 0.97872
Diffraction limits [Å] 1.756 1.756 1.677
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 0.894 a^* - 0.447 b^*
Direction-2 b^*
Direction-3 c^*
Anomalous signal up to 5.5 Å

	Overall	Inner Shell	Outer Shell
Low resolution limit	54.900	54.900	1.780
High resolution limit	1.701	4.832	1.701
Rmerge (all I+ & I-)	0.055	0.031	1.147
Rmeas (all I+ & I-)	0.059	0.033	1.238
Rpim (all I+ & I-)	0.022	0.012	0.463
Total number of observations	608799	28937	28754
Total number unique	83442	4172	4175
Mean(I)/sd(I)	17.6	47.9	1.4
Completeness (spherical)	90.8	99.9	35.7
Completeness (ellipsoidal)	95.4	99.9	56.0
Multiplicity	7.3	6.9	6.9
CC(1/2)	0.999	0.999	0.596
Anomalous completeness (spherical)	90.7	99.6	35.5
Anomalous completeness (ellipsoidal)	95.4	99.6	56.0
Anomalous multiplicity	3.7	3.7	3.5
CC(ano)	0.078	0.182	-0.025
DANO /sd(DANO)	0.756	1.059	0.619

Final scaling/merging - anisotropic data analysis via STARANISO

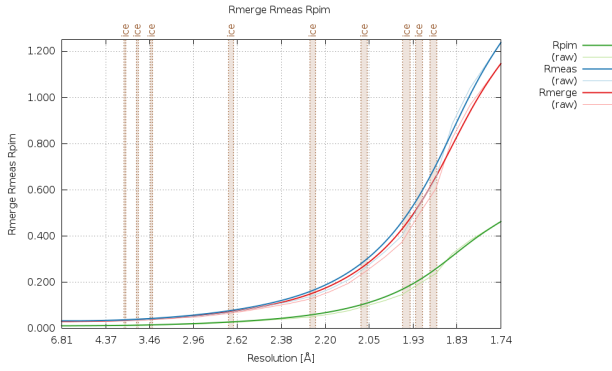


Fig.1 : R-values as a function of resolution (observations)

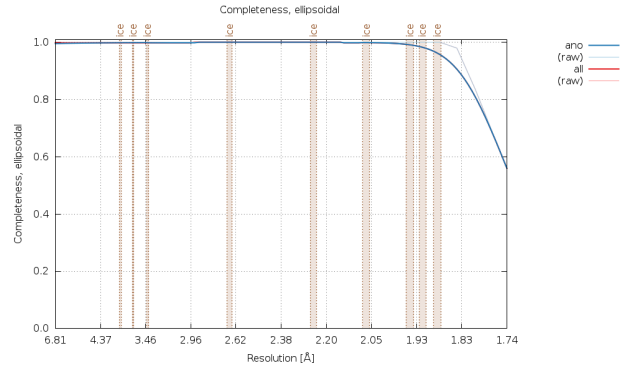


Fig.2 : Completeness (ellipsoidal) as a function of resolution (observations) - this is the relevant value here.

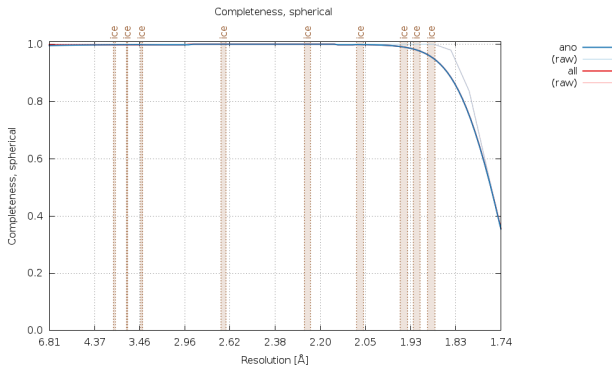


Fig.3 : Completeness (spherical) as a function of resolution (observations)

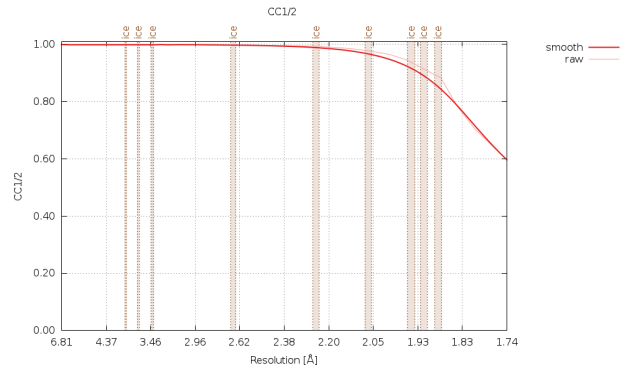


Fig.4 : CC1/2 as a function of resolution (observations)

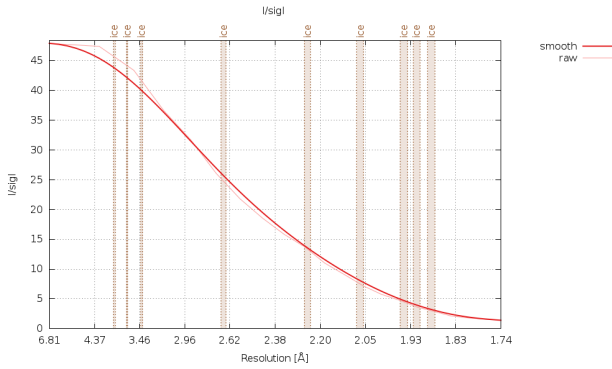


Fig.5 : I/sigI as a function of resolution (observations)

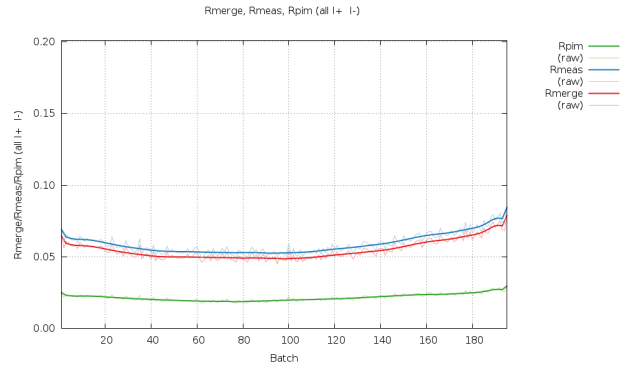


Fig.6 : R-values as a function of image number (observations)

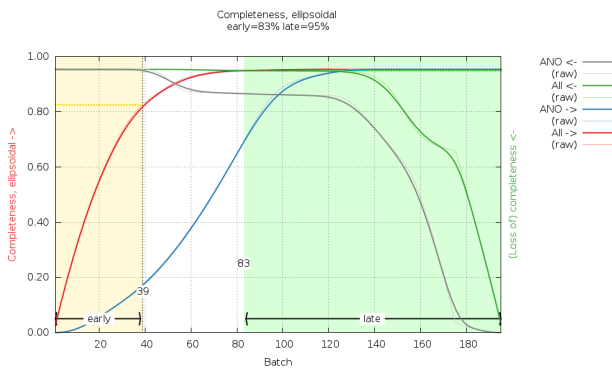


Fig.7 : Completeness (ellipsoidal) as a function of image number (observations) - this is the relevant value here.

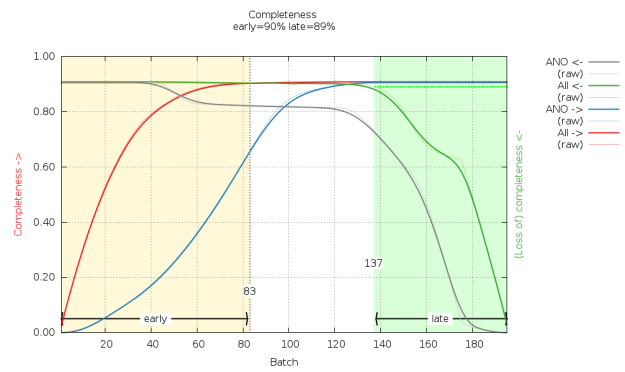


Fig.8 : Completeness (spherical) as a function of image number (observations)

Final scaling/merging - anisotropic data analysis via STARANISO

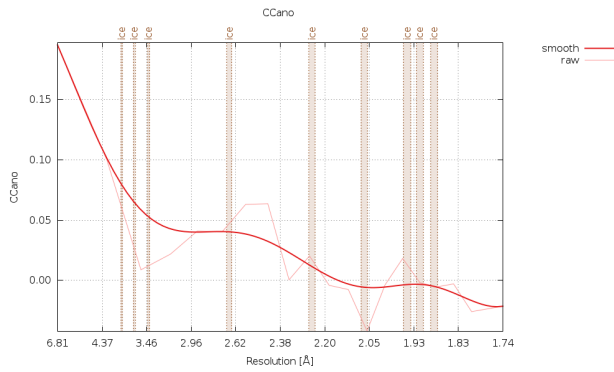


Fig.9 : CCano as a function of resolution (observations)

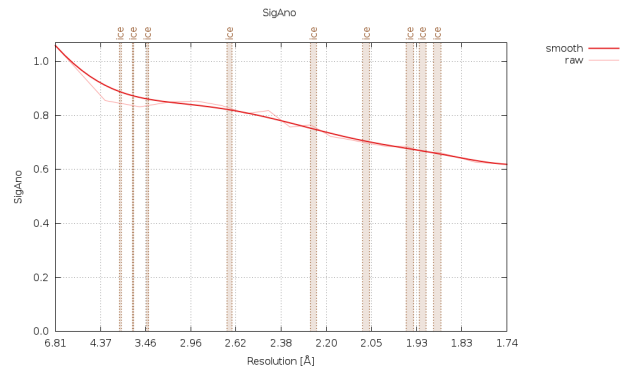


Fig.10 : SigAno as a function of resolution (observations)

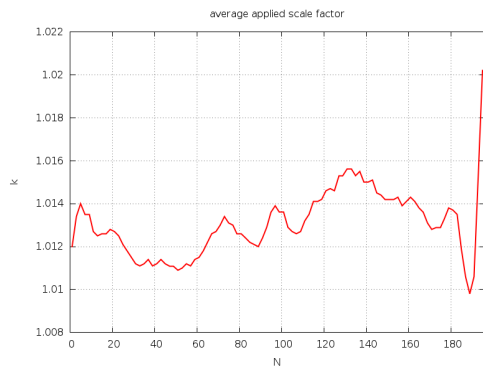


Fig.11 : Scale factor (isotropic AIMLESS scaling) as a function of image number (measurements)

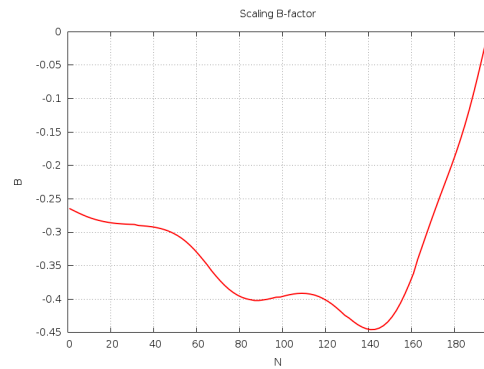


Fig.12 : Scaling B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

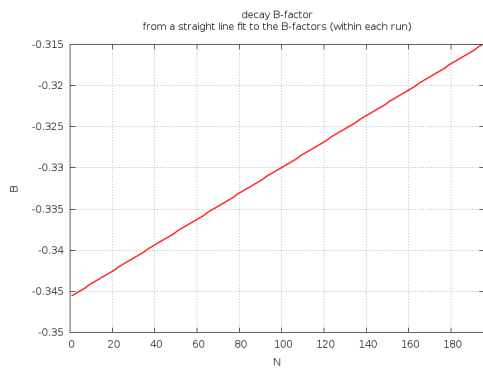


Fig.13 : Decay B-factor (isotropic AIMLESS scaling) as a function of image number (measurements)

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

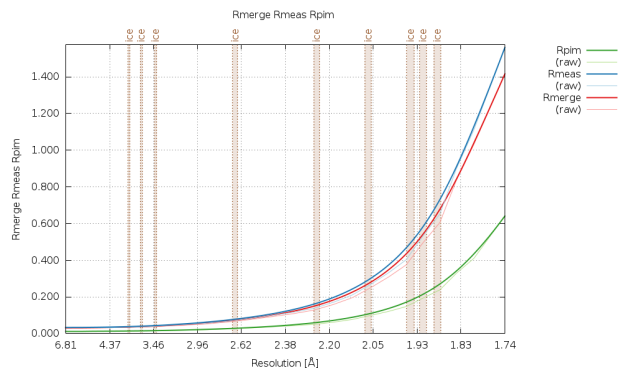


Fig.14 : R-values as a function of resolution (measurements)

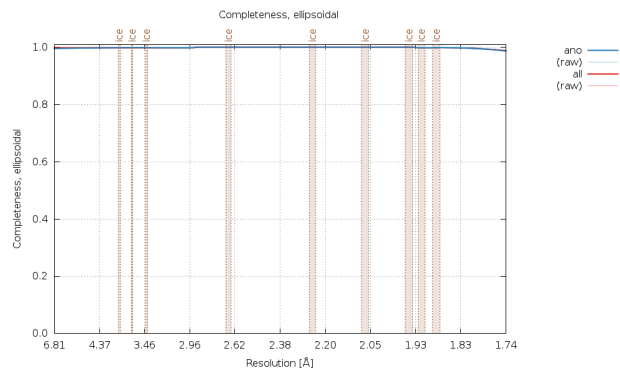


Fig.15 : Completeness (ellipsoidal) as a function of resolution (measurements)

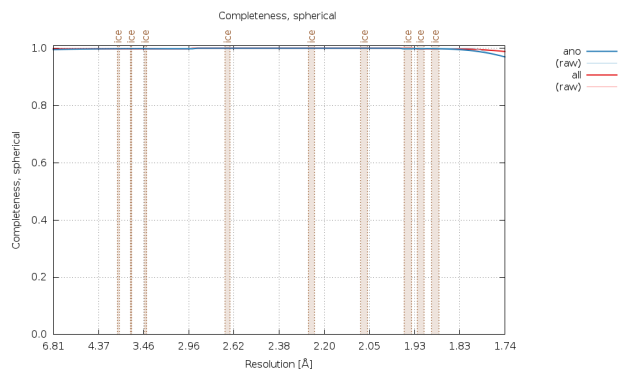


Fig.16 : Completeness (spherical) as a function of resolution (measurements)

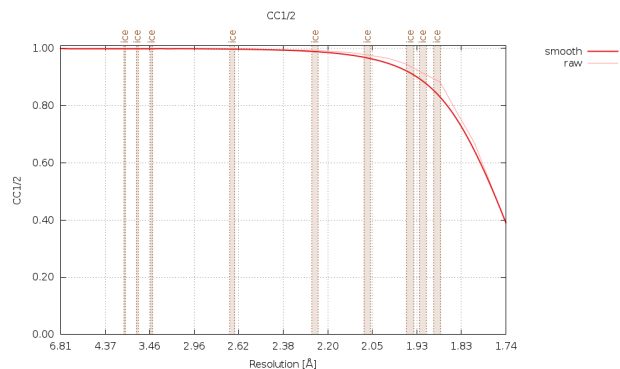


Fig.17 : CC1/2 as a function of resolution (measurements)

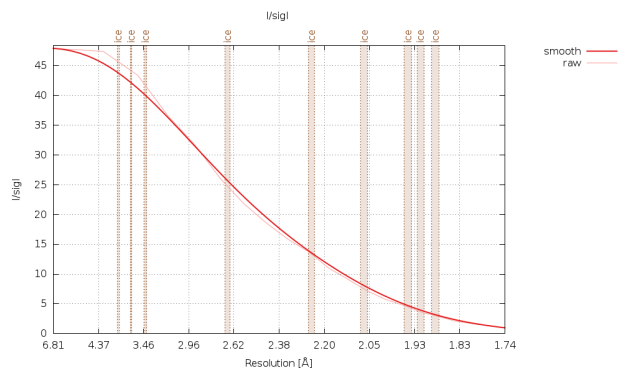


Fig.18 : I/sigI as a function of resolution (measurements)

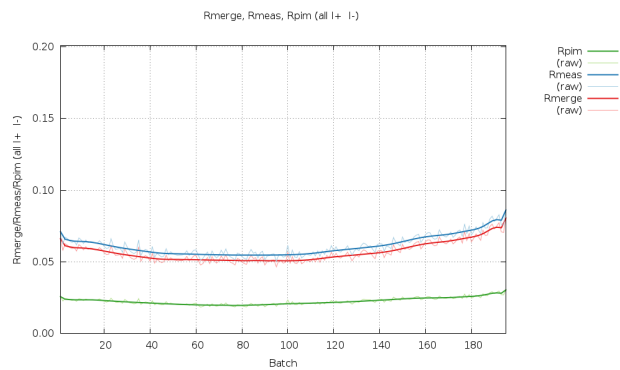


Fig.19 : R-values as a function of image number (measurements)

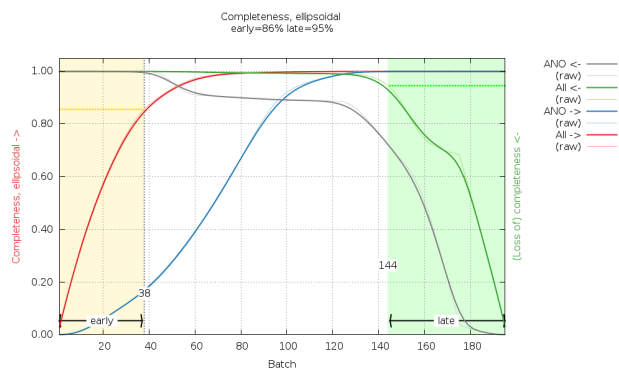


Fig.20 : Completeness (ellipsoidal) as a function of image number (measurements)

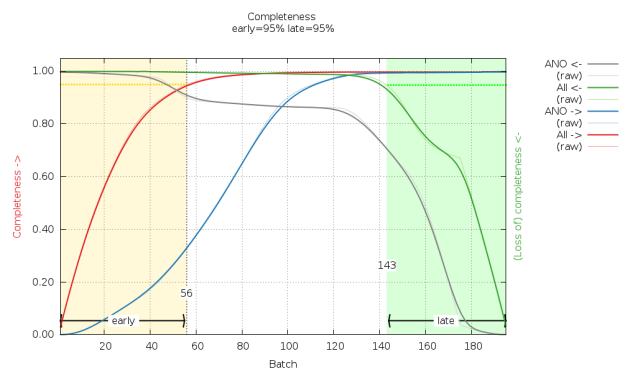


Fig.21 : Completeness (spherical) as a function of image number (measurements)

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

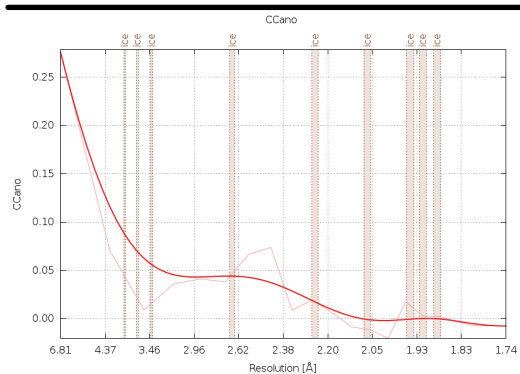


Fig.22 : CCano as a function of resolution (measurements)

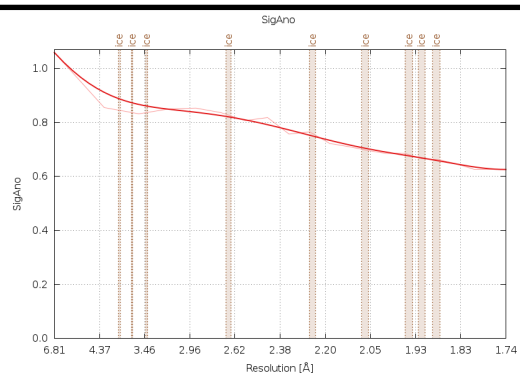


Fig.23 : SigAno as a function of resolution (measurements)

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. (2020). STARANISO. Cambridge, United Kingdom: Global Phasing Ltd.