ISPyB related work at Global Phasing

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MXCube/ISPyB Meeting
DLS
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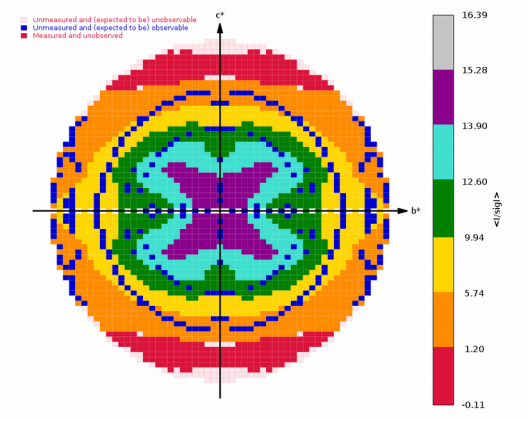
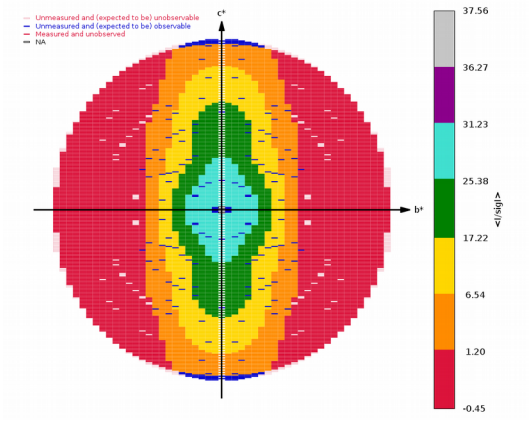
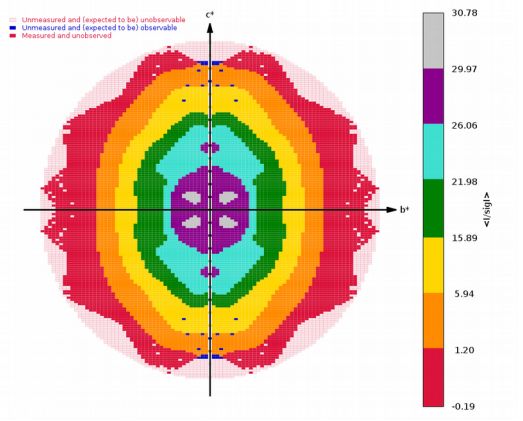
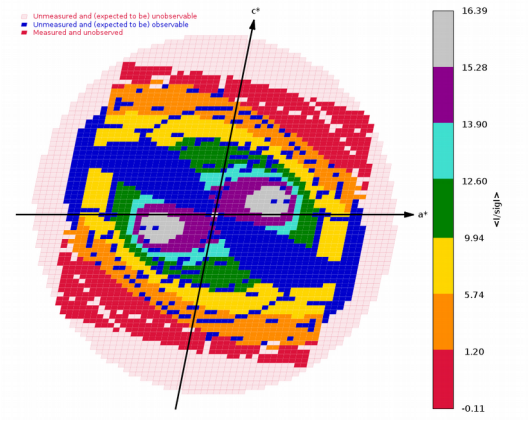
STARANISO

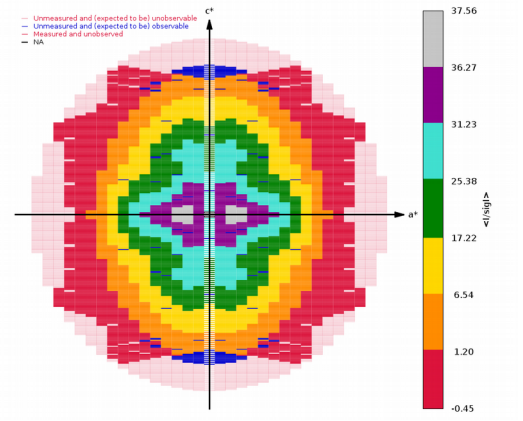








Plots of local <I/sigI> for each r.l.p.



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autoPROC: merging statistics

- autoPROC creates two types of merged data:
  - traditional (isotropic) analysis of high-resolution limit: truncate.mtz
  - new anisotropic analysis with STARANISO: staraniso_alldata.mtz
- we tried to make it much clearer, what statistics relate to what output (merged) reflection data – especially in summary.html
- because autoPROC supports processing of multi-sweep datasets, these statistics are potentially given multiple times (per-sweep and final merging)
- since summary.html is also intended as a procedural record, statistics are given both during the scaling step and again at the end (producing final MTZ files)
- … hopefully, this is not too confusing (we used colour to highlight different types)

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autoPROC: “table 1” - traditional

2.7. Finalising

Output file created (classical isotropic treatment of data) = truncate-unique.mtz

Spacegroup name P21
Unit cell parameters 50.68 89.80 60.47 90.000 94.778 90.000
Wavelength 0.97940 A

	Overall	InnerShell	OuterShell
Low resolution limit	89.800	89.800	1.970
High resolution limit	1.937	5.258	1.937
Rmerge (all I+ & I-)	0.104	0.055	0.637
Rmerge (within I+/I-)	0.089	0.039	0.610
Rmeas (within I+/I-)	0.122	0.054	0.831
Rmeas (all I+ & I-)	0.124	0.066	0.751
Rpim (within I+/I-)	0.083	0.038	0.561
Rpim (all I+ & I-)	0.066	0.036	0.394
Total number of observations	127299	6404	6869
Total number unique	37680	1951	1947
Mean(I)/sd(I)	9.1	20.6	2.3
Completeness	93.8	94.1	98.0
Multiplicity	3.4	3.3	3.5
CC(1/2)	0.994	0.992	0.796
Anomalous completeness	83.2	84.2	86.3
Anomalous multiplicity	1.8	1.8	1.9
CC(ano)	0.121	0.479	0.090
|DANO|/sd(DANO)	0.890	1.402	0.772

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autoPROC: “table 1” - anisotropic

Final output file created (including analysis of anisotropy via STARANISO) = staraniso_alldata.mtz (see above for detailed analysis of anisotropy)

```
Spacegroup name          P21
Unit cell parameters     50.68 89.80 60.47 90.000 94.778 90.000
Wavelength               0.97940 A

Resolution limits & eigenvectors of ellipsoid fitted to resolution cut-off surface:
  2.163         0.9996   0.0000   0.0279       0.998 _a_* - 0.066 _c_*
  1.658         0.0000   1.0000   0.0000       _b_*
  1.647        -0.0279   0.0000   0.9996      -0.023 _a_* + _c_*

                                            Overall  InnerShell  OuterShell
-------------------------------------------------------------------------------
   Low resolution limit                      89.800      89.800       1.761
   High resolution limit                      1.647       5.075       1.647


   Rmerge  (all I+ & I-)                      0.108       0.055       0.911
   Rmerge  (within I+/I-)                     0.093       0.039       1.034
   Rmeas   (within I+/I-)                     0.127       0.054       1.290
   Rmeas   (all I+ & I-)                      0.129       0.066       1.082
   Rpim    (within I+/I-)                     0.085       0.038       0.766
   Rpim    (all I+ & I-)                      0.069       0.035       0.576
   Total number of observations             143816        7084        7292
   Total number unique                       43159        2150        2143
   Mean(I)/sd(I)                               8.2        20.5         1.5
   Completeness (spherical)                   66.2        94.3        18.2
   Completeness (ellipsoidal)                 86.7        94.3        58.3
   Multiplicity                                3.3         3.3         3.4
   CC(1/2)                                   0.994       0.992       0.476


   Anomalous completeness (spherical)         56.1        84.7        13.1
   Anomalous completeness (ellipsoidal)       73.5        84.7        39.5
   Anomalous multiplicity                      1.8         1.8         1.9
   CC(ano)                                   0.112       0.410      -0.130
   |DANO|/sd(DANO)                           0.895       1.375       0.889
```

autoPROC: STARANISO XML

XML file written as 03/autoPROC.xml (for /home/vonrhein/Projects/JCSG/20170616/Results/4LII/177823/03/truncate-unique.mtz)

isotropic analysis

XML file written as 03/autoPROC_staraniso.xml (for /home/vonrhein/Projects/JCSG/20170616/Results/4LII/177823/03/staraniso_alldata-unique.mtz)

STARANISO mtz file (result)

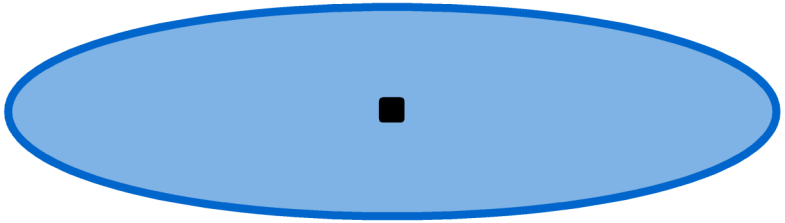
all following statistics are based on **observations** (as defined by STARANISO)

autoPROC: STARANISO XML

autoPROC_staraniso.xml

Node	Content
xml	version="1.0"
AutoProcContainer	
AutoProcProgramContainer	
AutoProc	
AutoProcScalingContainer	
AutoProcScaling	
recordTimeStamp	2017-06-19 10:47:17
StaranisoEllipsoid	
StaranisoEllipsoidRotationMatrix	
StaranisoEllipsoidRotationMatrix11	1.00000
StaranisoEllipsoidRotationMatrix12	.00000
StaranisoEllipsoidRotationMatrix13	.00000
StaranisoEllipsoidRotationMatrix21	.00000
StaranisoEllipsoidRotationMatrix22	1.00000
StaranisoEllipsoidRotationMatrix23	.00000
StaranisoEllipsoidRotationMatrix31	.00000
StaranisoEllipsoidRotationMatrix32	.00000
StaranisoEllipsoidRotationMatrix33	1.00000
StaranisoEllipsoidEigenvalues	
StaranisoEllipsoidEigenvalue1	2.15500
StaranisoEllipsoidEigenvalue2	2.37300
StaranisoEllipsoidEigenvalue3	1.92600
AutoProcScalingStatistics	
AutoProcScalingStatistics	

Design | Source



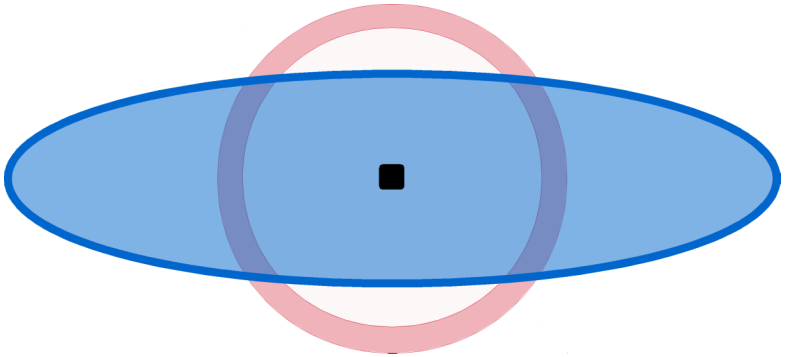
description of fitted ellipsoid
(including high-resolution limits)

autoPROC: STARANISO XML

autoPROC_staraniso.xml

Node	Content
StaranisoEllipsoidRotationMatrix32	.00000
StaranisoEllipsoidRotationMatrix33	1.00000
StaranisoEllipsoidEigenvalues	
StaranisoEllipsoidEigenvalue1	2.15500
StaranisoEllipsoidEigenvalue2	2.37300
StaranisoEllipsoidEigenvalue3	1.92600
AutoProcScalingStatistics	
scalingStatisticsType	overall
resolutionLimitLow	87.650
resolutionLimitHigh	1.928
rMerge	.153
rMeasWithinIPlusIMinus	.174
rMeasAllIPlusIMinus	.179
rPimWithinIPlusIMinus	.118
rPimAllIPlusIMinus	.092
nTotalObservations	191759
nTotalUniqueObservations	52422
meanIOverSigI	11.3
completenessSpherical	64.7
completenessEllipsoidal	87.0
completeness	64.7
multiplicity	3.7
ccHalf	.992
anomalousCompletenessSpherical	60.4
anomalousCompletenessEllipsoidal	82.2
anomalousCompleteness	60.4
anomalousMultiplicity	2.0
ccAnomalous	.033
DanoOverSigDano	.885
AutoProcScalingStatistics	
AutoProcScalingStatistics	

Design Source



spherical completeness (observations within shell compared to all possible reflections within spherical shell)

ellipsoidal completeness (observations within shell compared to possible reflections within that shell and within ellipsoid)

ditto for anomalous data