GΦL

Global Phasing Limited

The STARANISO Server

Anisotropy of the Diffraction Limit
and
Bayesian Estimation of Structure Amplitudes

Illicium verum

- **Your STARANISO job eocdgF42qmcTbhYV for 'temp-trunc_offset.ahkl' completed successfully.**

- **Select the color-coded reciprocal lattice scene(s) to view in WebGL 3-D:**

  ☐ **Experimental:** -log P(χ^2)　　☑ Redundancy　　☑ Mean $I/\sigma(I)$　　☑ Weighted CC½　　☐ Z(wCC½)　　☐ **Experimental:** Kullback-Leibler divergence　　☐ Cut-off surface　　☑ Debye-Waller factor

  | Check all | | VIEW Reciprocal lattices in WebGL |

  This uses our 3-D RLViewer tool (based on **WebGL** technology) within your browser - no external program or additional tool need be installed. Note that this opens the viewer in a new window, allowing it to be displayed side-by-side with the statistics on this page. To move a tabbed window to a separate browser instance: drag the tab in the tab bar **downwards** (not sideways) and release it where you want it placed (you can also drag it back).

  | Download outputs | Retrieve a previous job | Submit a new job |

- **Merging statistics table for observed data extracted from the final MRFANA log file:**

Resolution		#uniq	#Rfac	Rmerge	Rmeas	Rpim	#Isig	I/sigI	Compl. Spher. all	ano	Multiplicity all	ano	CC(1/2)	#CCAno	CC(ano)	SigAno	Compl. Ellip. all	ano
43.737 –	7.449	936	2358	0.043	0.052	0.029	936	18.506	0.5229	0.3742	2.68	1.62	0.9941	274	−0.1018	0.821	0.5229	0.3742
7.449 –	5.911	936	2221	0.062	0.077	0.044	936	12.089	0.5339	0.3164	2.57	1.66	0.9926	208	−0.0267	0.827	0.5339	0.3164
5.911 –	5.210	936	2197	0.070	0.086	0.049	936	11.109	0.5825	0.3453	2.55	1.64	0.9917	197	0.1731	0.786	0.5825	0.3453
5.210 –	4.768	937	2119	0.066	0.081	0.046	937	11.508	0.6006	0.3324	2.48	1.63	0.9909	176	−0.0150	0.794	0.6006	0.3324
4.768 –	4.415	935	2040	0.070	0.087	0.049	935	11.805	0.5452	0.2663	2.42	1.67	0.9907	159	−0.0728	0.815	0.5452	0.2663
4.415 –	4.169	937	2055	0.077	0.095	0.054	937	10.324	0.5893	0.3009	2.42	1.62	0.9918	157	0.2035	0.807	0.5893	0.3009
4.169 –	3.970	936	2094	0.088	0.109	0.063	936	9.569	0.6023	0.3043	2.45	1.65	0.9876	153	−0.0971	0.838	0.6023	0.3043
3.970 –	3.803	935	2068	0.116	0.145	0.084	935	7.837	0.6040	0.2980	2.43	1.63	0.9771	143	0.0013	0.834	0.6040	0.2980
3.803 –	3.658	936	2175	0.131	0.163	0.096	936	7.337	0.5756	0.2992	2.50	1.63	0.9747	144	0.0115	0.787	0.5756	0.2992
3.658 –	3.516	937	2171	0.148	0.184	0.107	937	6.690	0.5051	0.2323	2.49	1.69	0.9739	144	0.0221	0.783	0.5051	0.2323
3.516 –	3.390	936	2207	0.166	0.206	0.120	936	5.836	0.4919	0.2226	2.53	1.73	0.9706	144	0.0234	0.769	0.4945	0.2234
3.390 –	3.275	937	2260	0.200	0.249	0.145	937	5.402	0.4648	0.2094	2.56	1.72	0.9538	137	0.0467	0.763	0.4916	0.2211
3.275 –	3.171	936	2217	0.244	0.303	0.177	936	4.337	0.4570	0.1835	2.52	1.77	0.9320	139	−0.2009	0.726	0.4994	0.2080
3.171 –	3.076	936	2231	0.282	0.351	0.205	936	3.790	0.4386	0.1637	2.52	1.78	0.9197	142	0.1545	0.871	0.4856	0.1928
3.076 –	2.986	935	2178	0.325	0.407	0.241	935	3.047	0.4095	0.1396	2.47	1.79	0.8886	132	0.0547	0.752	0.4622	0.1679
2.986 –	2.900	937	2081	0.384	0.482	0.285	937	2.675	0.3812	0.1070	2.39	1.82	0.8724	114	0.1185	0.863	0.4250	0.1204
2.900 –	2.809	937	1981	0.393	0.498	0.299	937	2.355	0.3180	0.0650	2.30	1.86	0.8147	75	−0.0128	0.914	0.3220	0.0583
2.809 –	2.715	936	1975	0.420	0.538	0.329	936	2.166	0.2704	0.0433	2.28	1.95	0.7748	69	0.3299	0.924	0.2406	0.0228
2.715 –	2.615	936	1977	0.484	0.625	0.387	936	1.919	0.2208	0.0295	2.26	1.91	0.7243	49	0.1593	0.890	0.1672	0.0020
2.615 –	2.501	936	1927	0.645	0.846	0.540	936	1.392	0.1642	0.0189	2.20	1.75	0.5463	30	0.1671	0.939	0.1160	0.0000
Total: 43.737 –	2.501	18723	42532	0.102	0.127	0.074	18723	6.985	0.4089	0.1692	2.45	1.69	0.9917	2786	−0.0005	0.811	0.4567	0.2041

- **Merging statistics plots for observed data extracted from the MRFANA log file** (click image to enlarge):
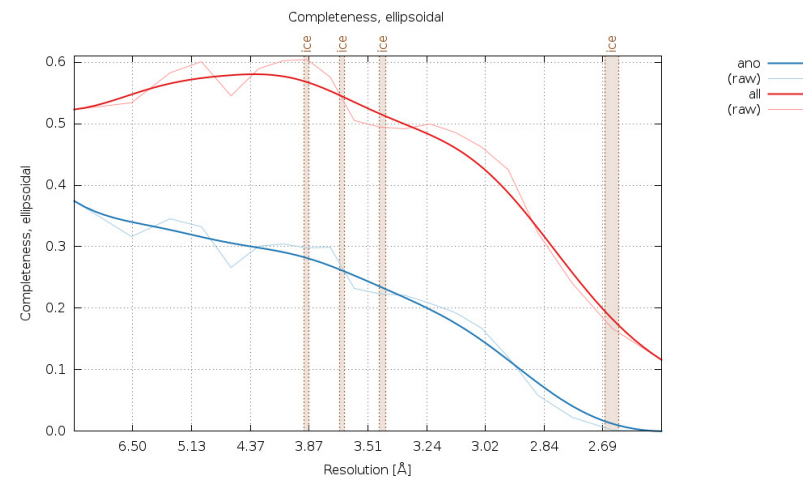
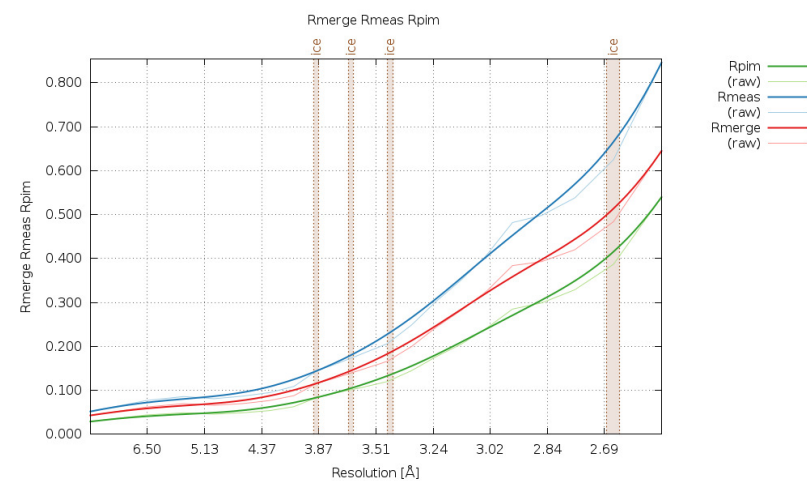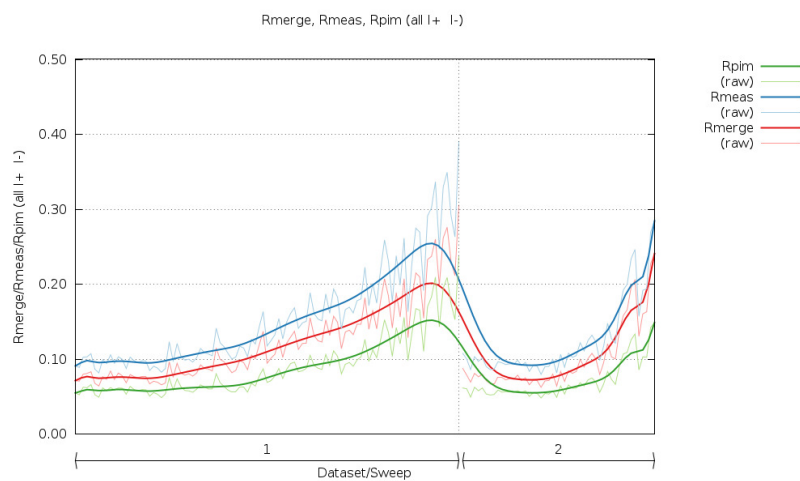Spherical completeness *vs.* image no.:
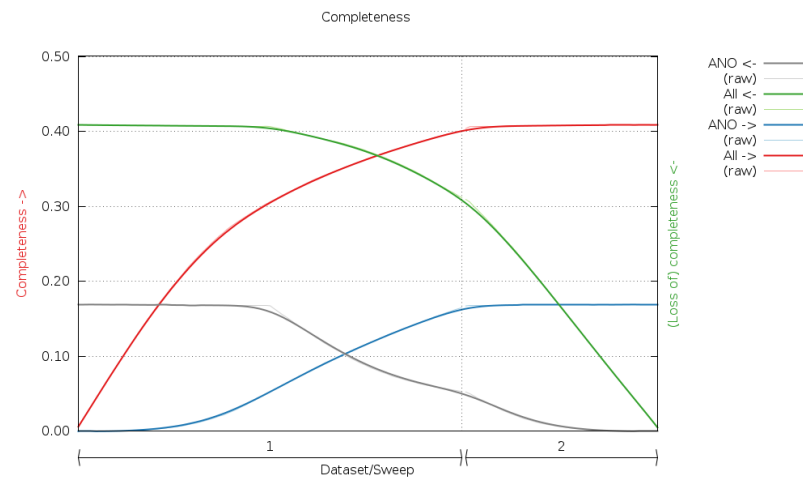
Spherical completeness *vs.* resolution (mean *d*-spacing):
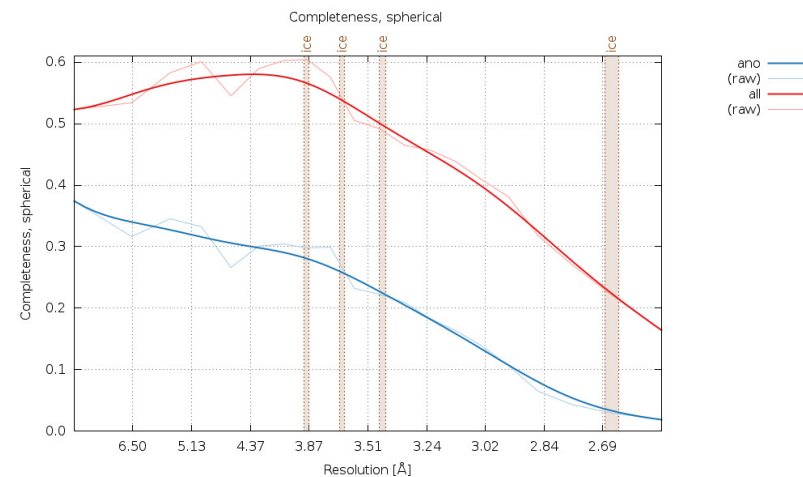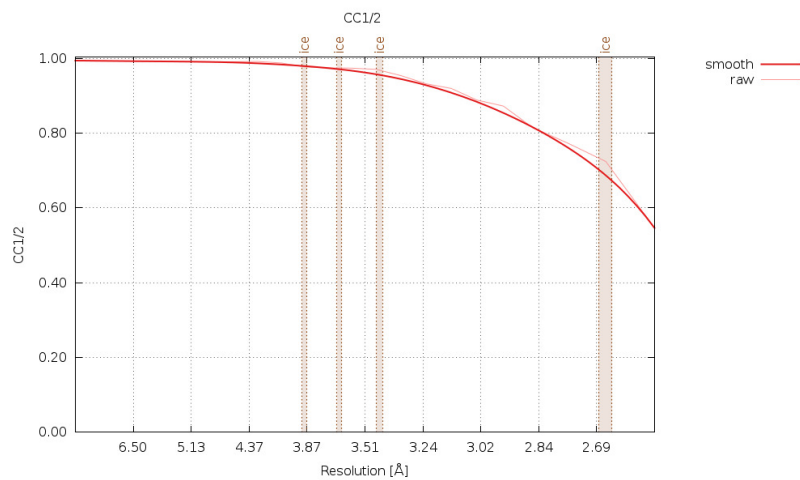

Ellipsoidal completeness *vs.* image no.:
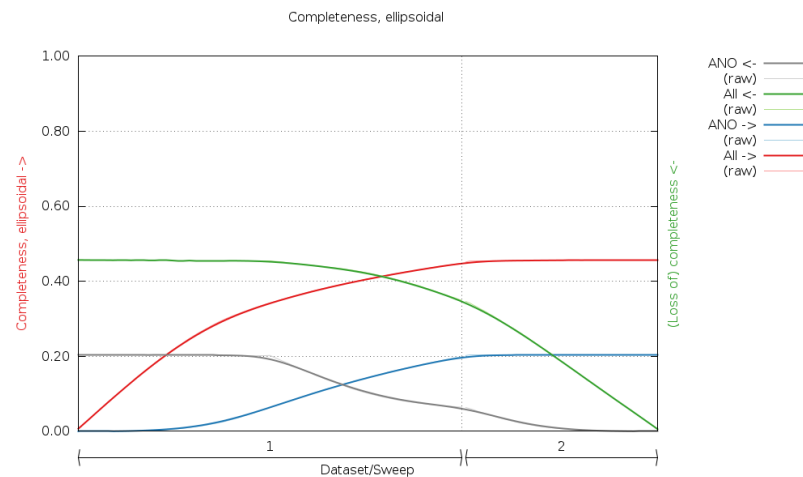
Ellipsoidal completeness *vs.* resolution:

Merging *R* values *vs.* image no.:

Merging *R* values *vs.* resolution:

Rmerge, Rmeas, Rpim (all I+ I-)

Rmerge Rmeas Rpim

CC$_{1/2}$ *vs.* resolution:

CC1/2

CC$_{1/2}$ano *vs.* resolution:

CCano
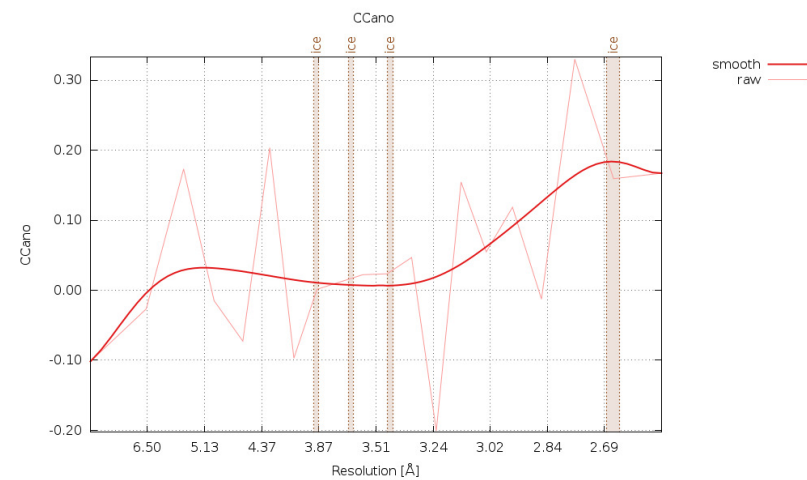
Mean $I/\sigma(I)$ *vs.* image no.:

Mean $I/\sigma(I)$ *vs.* resolution:
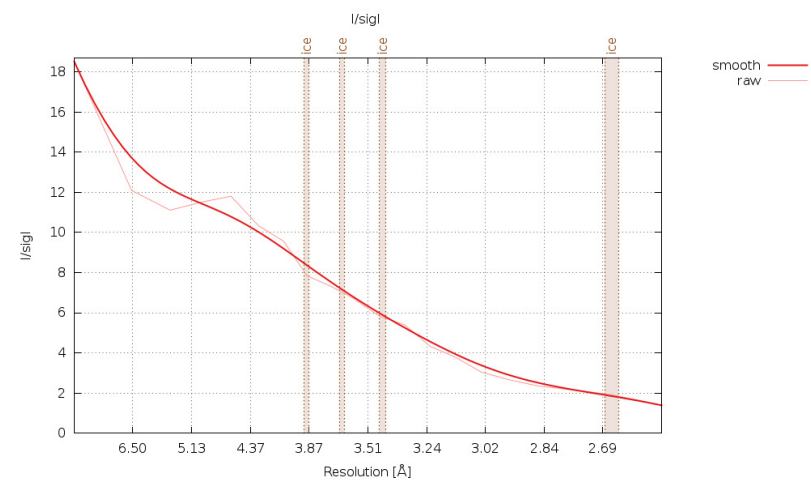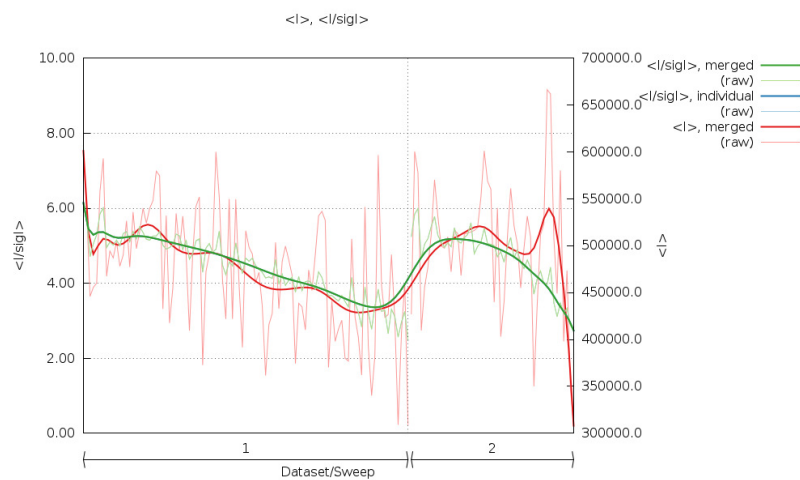
Mean Dano/$\sigma(D$ano$)$ *vs.* resolution:
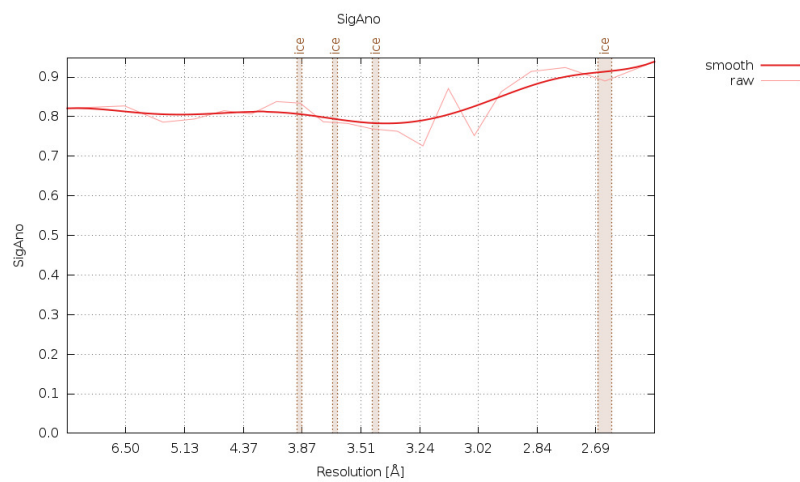
Spherical multiplicity (redundancy) *vs.* resolution:
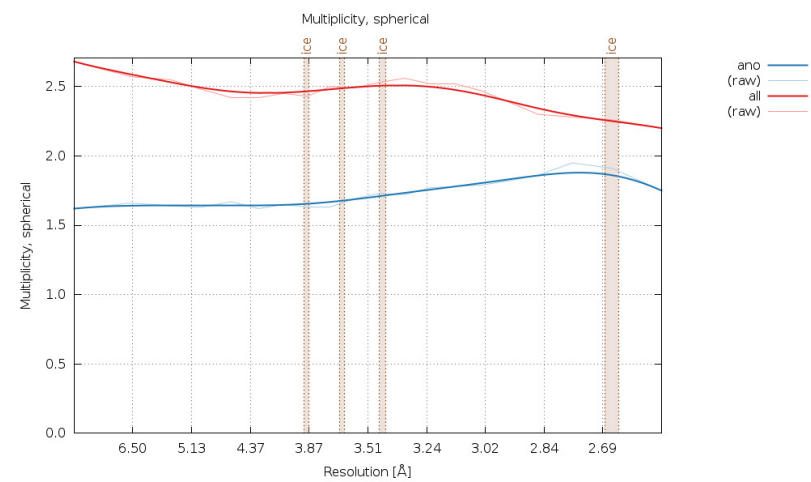
- **Summary of merging statistics for observed data:**

	Overall	InnerShell	OuterShell
Low resolution limit	43.737	43.737	2.615
High resolution limit	2.501	7.449	2.501
Rmerge (all I+ & I-)	0.102	0.043	0.645

```
Rmerge  (within I+/I-)                    0.087     0.038     0.596
Rmeas   (all I+ & I-)                     0.127     0.052     0.846
Rmeas   (within I+/I-)                    0.119     0.053     0.805
Rpim    (all I+ & I-)                     0.074     0.029     0.540
Rpim    (within I+/I-)                    0.080     0.036     0.535
Total number of observations            45903      2505      2062
Total number unique                     18723       936       936
Mean(I)/sd(I)                              7.0      18.5       1.4
Completeness (spherical)                  40.9      52.3      16.4
Completeness (ellipsoidal)                45.7      52.3      11.6
Multiplicity                               2.5       2.7       2.2
CC(1/2)                                   0.992     0.994     0.546

Anomalous completeness (spherical)        16.9      37.4       1.9
Anomalous completeness (ellipsoidal)      20.4      37.4       0.0
Anomalous multiplicity                     1.7       1.6       1.7
CC(ano)                                  -0.000    -0.102     0.167
|DANO|/sd(DANO)                           0.811     0.821     0.939
```

- **Data processing and anisotropy information extracted from the STARANISO log file:**

```
Using MTZ column labels:      IMEAN  SIGIMEAN  I(+)  SIGI(+)  I(-)  SIGI(-)  N(+)  N(-)  IHALF1  IHALF2

Unit cell and space group:    190.950 110.300  64.280  90.00  96.29  90.00   'C 1 2 1'
Nominal diffraction range:      43.737  2.501
Input reflection count:        28387

Diffraction cut-off criterion: Local mean I/sd(I) = 1.20

Diffraction limits & principal axes of ellipsoid fitted to diffraction cut-off surface:

                       3.432      0.7661  0.0000  0.6427      0.972 a* + 0.237 c*
                       2.237      0.0000  1.0000  0.0000            b*
                       2.482     -0.6427  0.0000  0.7661     -0.917 a* + 0.400 c*

GoF to ellipsoid (d*): 0.0415    Fraction of surface points fitted:  78.3% (    3511 /    4484)

Number of unobserved reflections inside ellipsoid:     6501
Number of observed reflections inside ellipsoid:      16168
Number of observed reflections outside ellipsoid:      2555

Lowest cut-off diffraction limit:
          3.991 at reflection   -7    3   16  in direction  -0.395 a* + 0.169 b* + 0.903 c*

Worst diffraction limit after cut-off:
         21.292 at reflection   -8    2    1  in direction  -0.963 a* + 0.241 b* + 0.120 c*

Best diffraction limit after cut-off:
          2.501 at reflection   52   30    5  in direction   0.863 a* + 0.498 b* + 0.083 c*

NOTE that because the cut-off surface is likely to be only very approximately ellipsoidal, in part
due to variations in reflection redundancy arising from the chosen collection strategy, the
directions of the worst and best diffraction limits may not correspond with the reciprocal axes,
even in high-symmetry space groups (the only constraint being that the surface must have point
symmetry at least that of the Laue class).

Fraction of data inside cut-off surface:      66.0% (   18723 /    28387)
```

Fraction of cut-off surface above threshold: 15.7% (234 /   1494)

WARNING: Diffraction of the input data has probably been truncated due to an inappropriate
(an)isotropic diffraction cut-off applied in previous processing, or the diffraction pattern may
have extended beyond the edges of the detector. In the latter case consider the possibilities of

either moving the detector closer or swinging it out, having carefully checked in the former case that this will not create a risk of spot overlap.

```
Fraction of total surface above threshold truncated by cusp(s):              55.4%  (   2481 /   4475)


Scale:                    5.117E-03   [ = factor to place Iobs on same scale as Iprofile/100.]
Beq:                         68.67    [ = equivalent overall isotropic B factor on Fs.]

                                B11     B22     B33     B23     B31     B12
Delta-B tensor:               -13.49  -22.50   35.99    0.00   -6.90    0.00
```

Note: the delta-B tensor is the overall anisotropy tensor on Fs after subtraction of Beq from its diagonal elements (so trace = 0).

Eigenvalues (E) & eigenvectors of overall anisotropy (B) tensor on Fs:

```
                54.24       0.9908   0.0000   0.1355       a* + 0.009 c*
                46.17       0.0000   1.0000   0.0000       b*
               105.61      -0.1355   0.0000   0.9908      -0.374 a* + 0.928 c*
```

The eigenvalues and eigenvectors of the overall B tensor are the squares of the lengths and the directions of the principal axes of the ellipsoid that represents the tensor.

```
Delta-B eigenvalues:              -14.44   -22.50    36.94
```

The delta-B eigenvalues are the eigenvalues of the overall anisotropy tensor after subtraction of Beq (so sum = 0).

Angle & axis of rotation of diffraction-limit ellipsoid relative to anisotropy tensor:

```
                32.20       0.0000  -1.0000   0.0000
```

```
Anisotropy ratio:          0.866   [ = (Emax - Emin) / Beq ]
Fractional anisotropy:     0.438   [ = sqrt(1.5 Sum_i (E_i - Beq)^2 / Sum_i E_i^2) ]
```

Eigenvalues & eigenvectors of redundancy anisotropy tensor:

```
                 1.20       0.9555   0.0000  -0.2951       0.990 a* - 0.139 c*
                 0.75       0.0000   1.0000   0.0000       b*
                 0.46       0.2951   0.0000   0.9555       0.691 a* + 0.723 c*
```

Eigenvalues & eigenvectors of mean I/sd(I) anisotropy tensor:

```
                 2.32       0.9900   0.0000  -0.1409       0.996 a* - 0.084 c*
                 1.62       0.0000   1.0000   0.0000       b*
                 1.00       0.1409   0.0000   0.9900       0.397 a* + 0.918 c*
```

Eigenvalues & eigenvectors of weighted CC_1/2 anisotropy tensor:

```
                0.367       0.9823   0.0000  -0.1873       0.995 a* - 0.100 c*
                0.284       0.0000   1.0000   0.0000       b*
                0.184       0.1873   0.0000   0.9823       0.503 a* + 0.864 c*
```

Eigenvalues & eigenvectors of Z(weighted CC_1/2) anisotropy tensor:

```
                59.77       0.9642   0.0000  -0.2651       0.992 a* - 0.128 c*
                42.78       0.0000   1.0000   0.0000       b*
                28.99       0.2651   0.0000   0.9642       0.646 a* + 0.763 c*
```

Eigenvalues & eigenvectors of mean K-L divergence anisotropy tensor:

```
                0.242       0.9891   0.0000  -0.1472       0.996 a* - 0.086 c*
                0.179       0.0000   1.0000   0.0000       b*
                0.112       0.1472   0.0000   0.9891       0.412 a* + 0.911 c*
```

Ranges of redundancy, local mean I/sd(I), local weighted CC_1/2, local Z(weighted CC_1/2), local mean K-L divergence and D-W factor [= exp(-4 pi^2 s~Us)]:

```
                    Redund  ISmean  CChalf  ZChalf  KLdive  DWfact
     0   Grey                       Unobservable*
     1   Blue                        Observable*
     2   Red|Pink:9      1    1.20  0.5000    45.00   0.193  0.0223
     3   Orange          2    4.04  0.8881   133.67   0.546  0.0660
     4   Yellow          3    9.57  0.9479   180.19   0.940  0.1628
     5   Green           5   14.14  0.9598   207.14   1.144  0.3347
     6   Cyan            6   18.18  0.9687   229.02   1.299  0.5740
     7   Magenta         7   22.35  0.9763   254.76   1.617  0.8212
     8   White           8   24.11  0.9791   268.35   2.059  0.9799


   * Refer to GLOSSARY for explanation of terminology.


   The cut-off surface uses a different color scheme:
   Unmeasured points are blue (inside the fitted surface) or cyan (outside).
   Unobserved points are red (in) or green (out).
   Observed points are orange (in) or white (out).
   The fitted surface is magenta.

   Anisotropic S/N ratio:         6.37     [ = max_h | exp(4 pi^2 s~_h delta(B) s_h) - 1 | <I_h/sd(I_h)> ]

   The 'anisotropic S/N ratio', unlike the 'anisotropy ratio' or the 'fractional anisotropy' shown
   above, in addition to the anisotropy of the B tensor, takes both the diffraction and the local mean
   I/sd(I) into account.
```

- **Instructions for using the reciprocal-lattice viewer (hit 'h' in viewer to see on-screen):**

  - **Mouse:**

Left-down & drag:	Rotate view.
Middle-down & drag:	Translate.
Right-down & drag:	Zoom.
Wheel:	Adjust z-clipping depth.
Left-down & wheel:	Adjust z-clipping position.

    Most of the mouse actions should also work on a touchscreen (*e.g.* tablet or smartphone), though a gesture to emulate the mousewheel may not be available on all devices!

  - **Keyboard:**

- =	Adjust point size.
0 .. 9	Toggle points in sets 0 (grey) to 9 (pink).
c	Reset only translation and z-clipping so that the objects are re-centred.
d	Toggle depth-cueing.
h	Toggle on-screen help text (all text can be resized by clicking anywhere in the caption text above the graphics canvas, then use Ctrl/Wheel).
i	Reset to initial orientation, translation, zoom and z-clipping.
n	Complement point visibilities.
p	Make screenshot (PNG): requires pop-ups from server to be allowed.
q	Stop/start rock/roll.
r	Cycle through rock, roll(-), roll(+).
s	Toggle d-spacing labels.
x	Reset orientation, translation and z-clipping to view down world x axis (initially to right).

y	Ditto for *y* axis (initially up).
z	Ditto for *z* axis (initially towards viewer).
Shift-x/y/z	View from negative axis direction.
Down/up arrow	Decrease/increase rocking amplitude.
Left/right arrow	Decrease/increase rock/roll speed.

- **IMPORTANT NOTE**

  If you don't see in the local mean $I/\sigma(I)$ plot at least a thin layer of **red** points (*i.e.* representing rejected data) that covers most of an outer **orange** spherical or ellipsoidal surface (representing the diffraction limit of observed significant data, (*i.e.* ignore any **dark blue** points representing unmeasured data), it means either that there were good data beyond the edges of the detector, or (more likely) that the advice concerning the application of a diffraction cut-off to the data prior to running STARANISO was not heeded. This should also have shown up as a warning in the summary of the anisotropy information extracted from the STARANISO log file above.

- **Select the color-coded reciprocal lattice scene(s) to view in WebGL 3-D:**

  ☐ **Experimental:** -log P(χ^2) ☑ Redundancy ☑ Mean $I/\sigma(I)$ ☑ Weighted CC½ ☐ Z(wCC½) ☐ **Experimental:** Kullback-Leibler divergence ☐ Cut-off surface ☑ Debye-Waller factor

  <div align="center">

  Check all   VIEW Reciprocal lattices in WebGL

  Download outputs   Retrieve a previous job   Submit a new job

  STARANISO server release v3.317 28-Apr-2020.

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