

The STARANISO Server
Anisotropy of the Diffraction Limit
and
Bayesian Estimation of Structure Amplitudes



- Your STARANISO job **cLDhZJ1an4c6wZ94** for '**temp-trunc_offset.ahkl**' completed successfully.

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

☐ Experimental: $-\log P(\chi^2)$ ☒ Redundancy ☒ Mean $I/\sigma(I)$ ☒ Weighted $CC\frac{1}{2}$ ☐ $Z(wCC\frac{1}{2})$ ☐ 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).

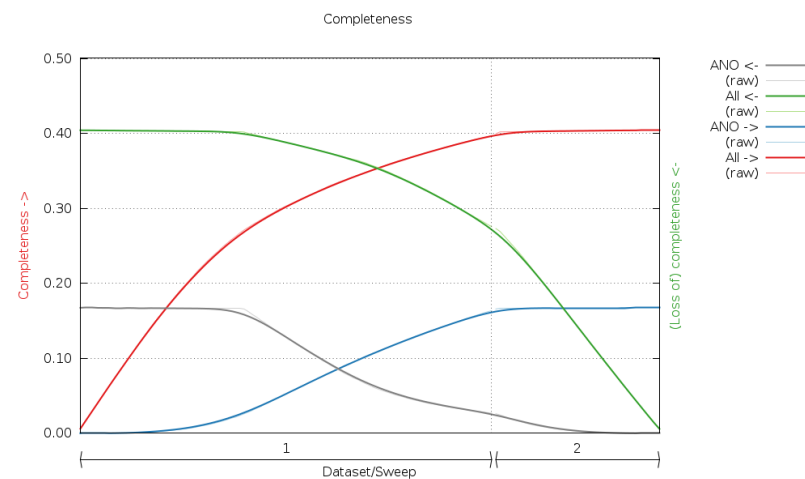
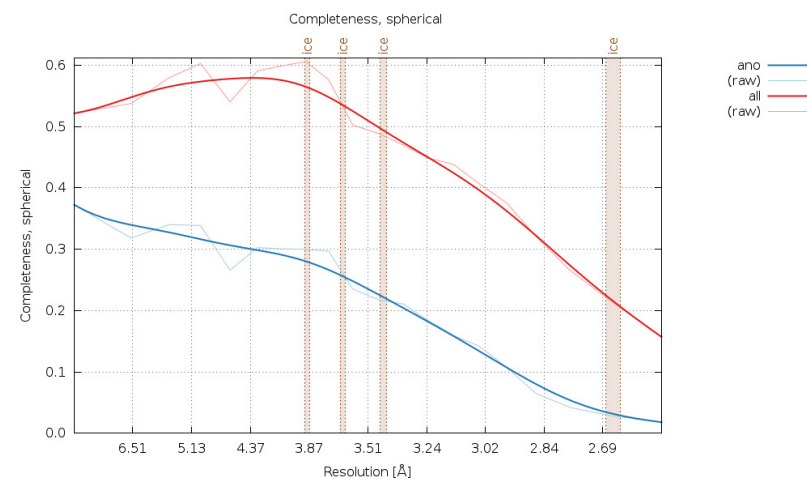
[Download outputs](#)[Retrieve a previous job](#)[Submit a new job](#)

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

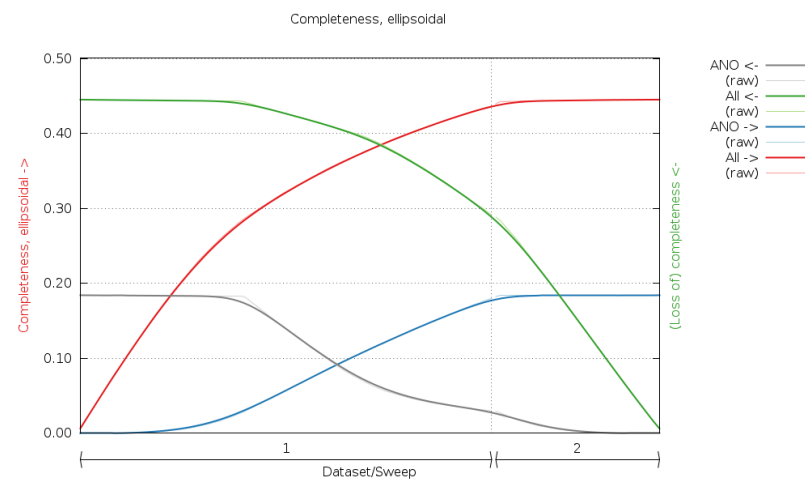
									Compl. Spher.		Multiplicity						Compl. Ellip.	
Resolution		#uniq	#Rfac	Rmerge	Rmeas	Rpim	#Isig	I/sigI	all	ano	all	ano	CC(1/2)	#CCAno	CC(ano)	SigAno	all	ano
41.748	- 7.466	925	2154	0.038	0.048	0.028	925	19.402	0.5214	0.3724	2.49	1.50	0.9962	202	0.0609	0.824	0.5214	0.3724
7.466	- 5.942	924	2012	0.058	0.073	0.043	924	12.396	0.5375	0.3183	2.39	1.52	0.9930	149	0.0066	0.810	0.5375	0.3183
5.942	- 5.233	925	1987	0.065	0.082	0.049	925	11.163	0.5796	0.3401	2.36	1.50	0.9919	129	0.1133	0.773	0.5796	0.3401
5.233	- 4.787	925	1948	0.060	0.076	0.045	925	11.737	0.6026	0.3386	2.34	1.50	0.9918	118	-0.1645	0.791	0.6026	0.3386
4.787	- 4.430	925	1841	0.065	0.082	0.049	925	12.064	0.5403	0.2659	2.25	1.52	0.9916	100	0.2706	0.844	0.5403	0.2659
4.430	- 4.184	923	1849	0.070	0.088	0.052	923	10.554	0.5909	0.3027	2.26	1.49	0.9917	94	0.0629	0.790	0.5909	0.3027
4.184	- 3.983	926	1878	0.083	0.105	0.063	926	9.698	0.5990	0.3007	2.27	1.49	0.9881	86	-0.0673	0.846	0.5990	0.3007
3.983	- 3.818	925	1922	0.108	0.138	0.083	925	8.090	0.6058	0.2999	2.30	1.51	0.9785	90	-0.0308	0.817	0.6058	0.2999
3.818	- 3.672	924	1940	0.122	0.155	0.093	924	7.319	0.5761	0.2966	2.32	1.49	0.9744	80	-0.0703	0.758	0.5761	0.2966
3.672	- 3.528	925	1946	0.136	0.172	0.104	925	6.817	0.5024	0.2351	2.31	1.53	0.9734	83	0.1685	0.764	0.5024	0.2351
3.528	- 3.401	925	1994	0.155	0.195	0.117	925	6.025	0.4889	0.2181	2.35	1.57	0.9697	79	0.1820	0.759	0.4882	0.2149
3.401	- 3.287	925	2032	0.190	0.240	0.144	925	5.366	0.4703	0.2108	2.38	1.58	0.9515	79	0.2211	0.740	0.4623	0.1882
3.287	- 3.182	924	2014	0.229	0.288	0.172	924	4.413	0.4485	0.1838	2.37	1.62	0.9358	81	-0.2016	0.717	0.4426	0.1457
3.182	- 3.087	925	2007	0.266	0.336	0.202	925	3.781	0.4382	0.1596	2.35	1.65	0.9162	75	0.0169	0.851	0.4308	0.1117
3.087	- 2.997	924	1985	0.304	0.385	0.233	924	3.078	0.4065	0.1418	2.33	1.65	0.8946	75	0.0236	0.727	0.3928	0.0872
2.997	- 2.908	926	1899	0.345	0.439	0.267	926	2.682	0.3757	0.1078	2.26	1.68	0.8864	67	0.1544	0.800	0.3508	0.0593
2.908	- 2.819	924	1742	0.387	0.493	0.300	924	2.309	0.3205	0.0647	2.14	1.76	0.8151	61	0.2275	0.916	0.3055	0.0294
2.819	- 2.723	925	1789	0.387	0.498	0.306	925	2.202	0.2653	0.0421	2.17	1.85	0.7872	58	0.2286	0.898	0.2523	0.0094
2.723	- 2.621	925	1805	0.468	0.610	0.383	925	1.873	0.2159	0.0287	2.15	1.80	0.7178	38	0.0613	0.845	0.2059	0.0019
2.621	- 2.502	925	1804	0.610	0.804	0.517	925	1.405	0.1570	0.0181	2.13	1.65	0.5688	21	0.1103	0.922	0.1665	0.0000
Total:	41.748 - 2.502	18495	38548	0.096	0.121	0.073	18495	7.119	0.4044	0.1675	2.30	1.56	0.9925	1765	0.0535	0.798	0.4453	0.1843

- Merging statistics plots for observed data extracted from the MRFANA log file (click image to enlarge):

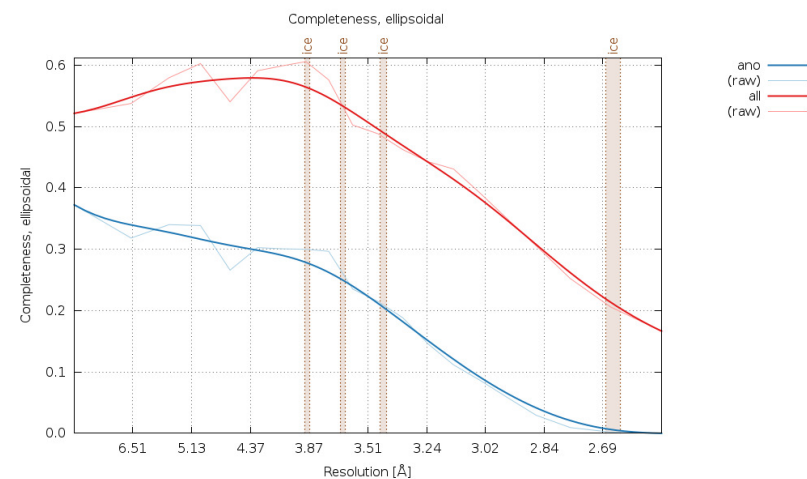
Spherical completeness vs. image no.:

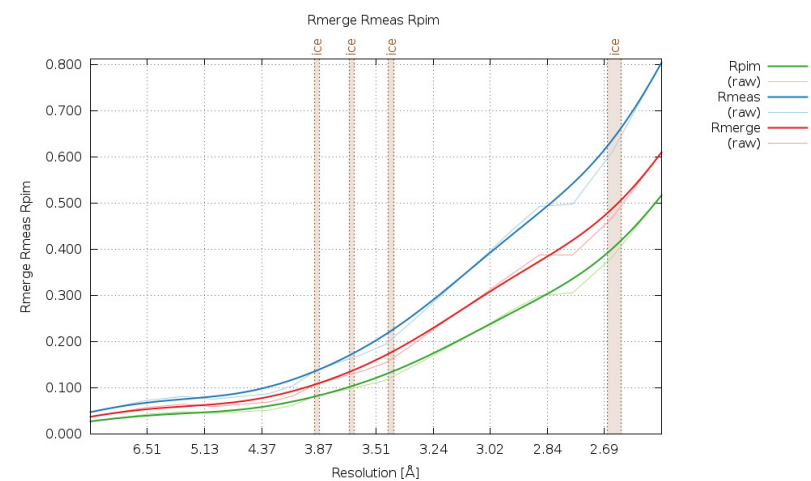
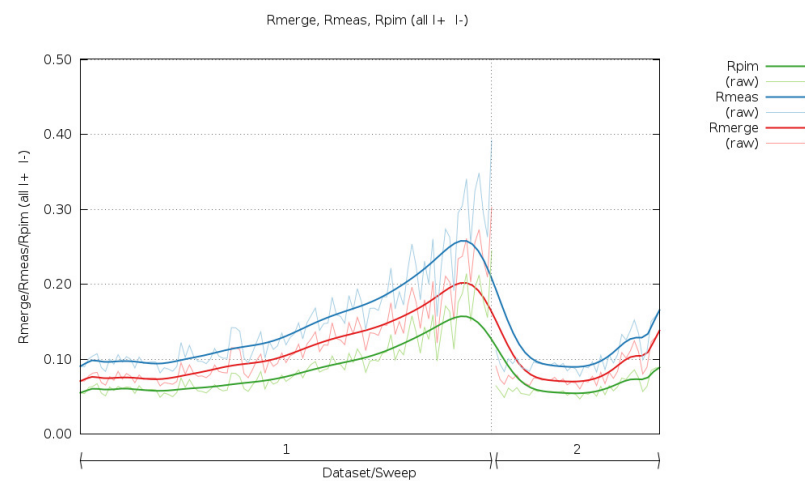
Spherical completeness vs. resolution (mean d -spacing):

Ellipsoidal completeness vs. image no.:

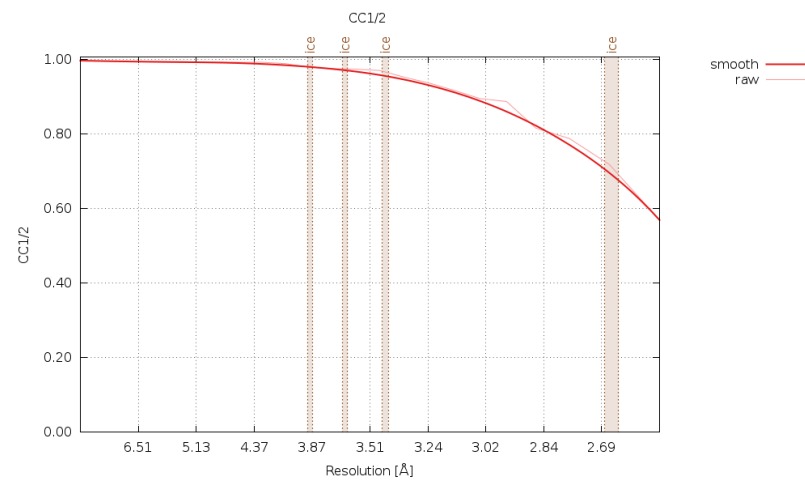


Ellipsoidal completeness vs. resolution:

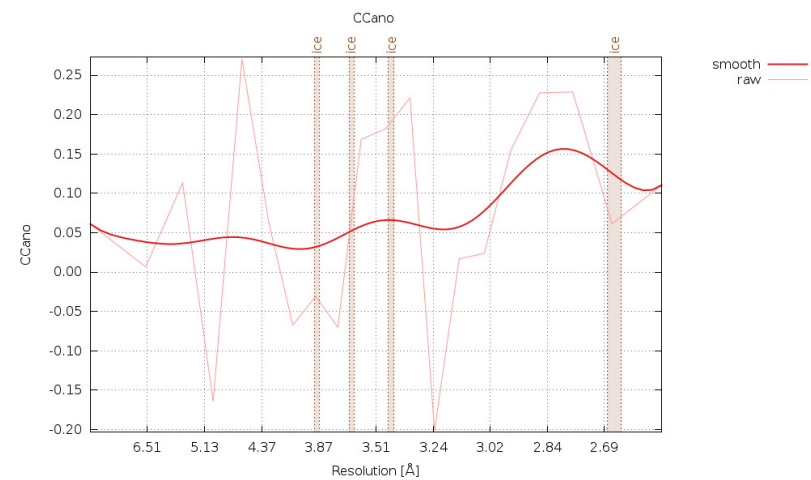
Merging R values vs. image no.:Merging R values vs. resolution:



CC_{1/2} vs. resolution:

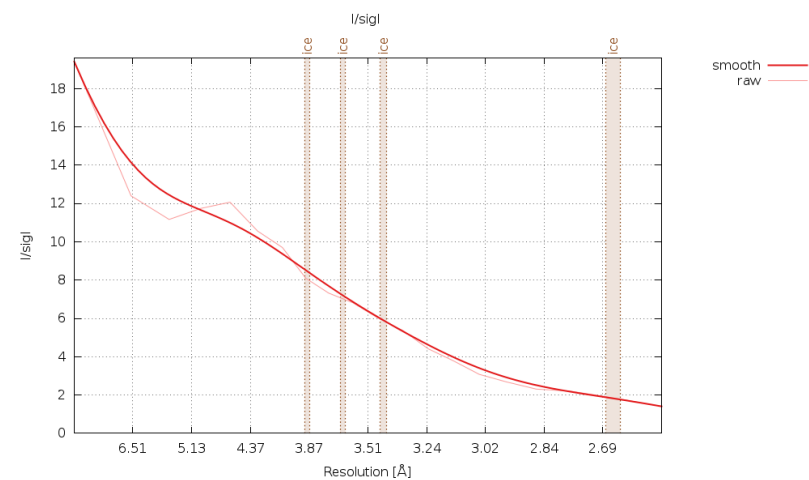
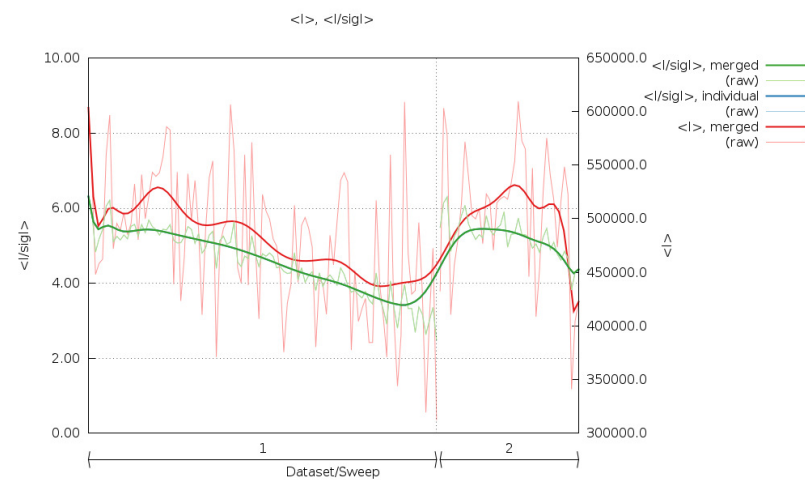
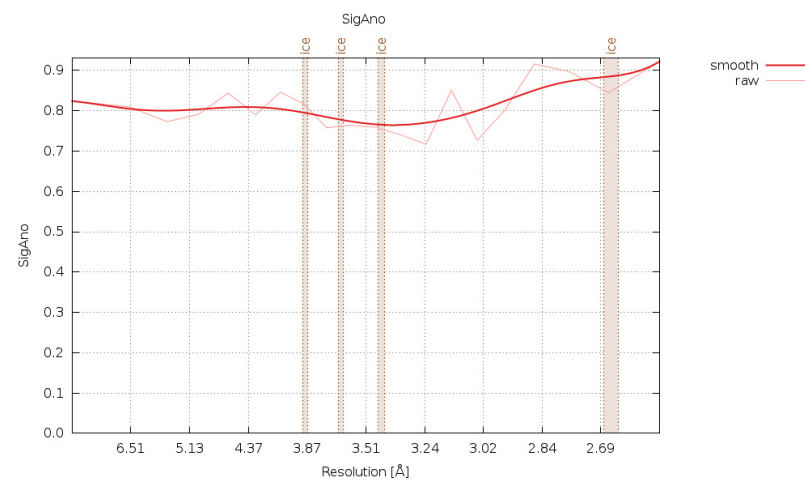


CC_{1/2}ano vs. resolution:

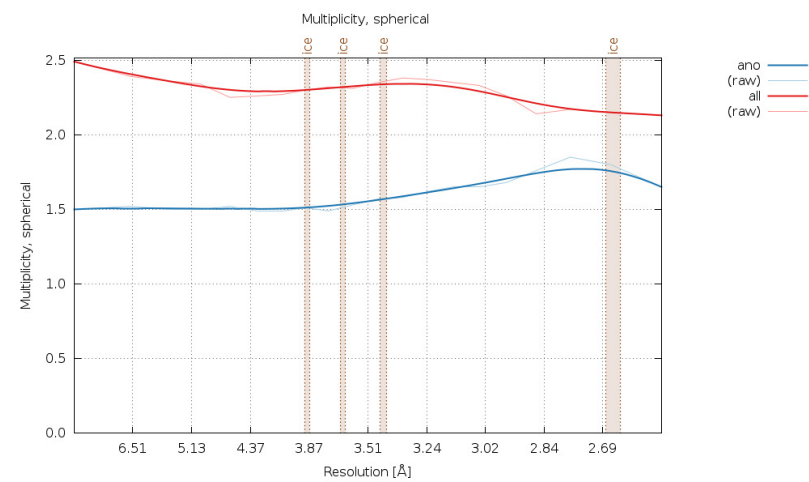


Mean $I/\sigma(I)$ vs. image no.:

Mean $I/\sigma(I)$ vs. resolution:

Mean $Dano/\sigma(Dano)$ vs. resolution:

Spherical multiplicity (redundancy) vs. resolution:

**Summary of merging statistics for observed data:**

	Overall	InnerShell	OuterShell
Low resolution limit	41.748	41.748	2.621
High resolution limit	2.502	7.466	2.502
Rmerge (all I+ & I-)	0.096	0.038	0.610

Rmerge (within I+/I-)	0.081	0.035	0.566
Rmeas (all I+ & I-)	0.121	0.048	0.804
Rmeas (within I+/I-)	0.111	0.048	0.764
Rpim (all I+ & I-)	0.073	0.028	0.517
Rpim (within I+/I-)	0.075	0.033	0.509
Total number of observations	42480	2307	1973
Total number unique	18495	925	925
Mean(I)/sd(I)	7.1	19.4	1.4
Completeness (spherical)	40.4	52.1	15.7
Completeness (ellipsoidal)	44.5	52.1	16.7
Multiplicity	2.3	2.5	2.1
CC(1/2)	0.992	0.996	0.569
Anomalous completeness (spherical)	16.8	37.2	1.8
Anomalous completeness (ellipsoidal)	18.4	37.2	0.0
Anomalous multiplicity	1.6	1.5	1.6
CC(ano)	0.054	0.061	0.110
DANO /sd(DANO)	0.798	0.824	0.922

• 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:    41.748  2.502
Input reflection count:       28366
```

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

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

3.479	0.7217	0.0000	-0.6922	0.942	a* - 0.337	c*
2.233	0.0000	1.0000	0.0000	b*		
2.456	0.6922	0.0000	0.7217	0.955	a* + 0.298	c*

GoF to ellipsoid (d*): 0.0422 Fraction of surface points fitted: 91.6% (4088 / 4465)

```
Number of unobserved reflections inside ellipsoid: 3672
Number of observed reflections inside ellipsoid: 15644
Number of observed reflections outside ellipsoid: 2851
```

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:
2.502 at reflection -76 4 3 in direction -0.998 **a*** + 0.053 **b*** + 0.039 **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: 65.2% (18495 / 28366)

Fraction of cut-off surface above threshold: 14.9% (221 / 1480)

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): 55.1% (2457 / 4461)

Scale: 5.178E-03 [= factor to place Iobs on same scale as Iprofile/100.]
Beq: 68.02 [= equivalent overall isotropic B factor on Fs.]

	B11	B22	B33	B23	B31	B12
Delta-B tensor:	-13.32	-21.88	35.20	0.00	-6.97	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:

53.72	0.9902	0.0000	0.1395	a* + 0.010 c*
46.14	0.0000	1.0000	0.0000	b*
104.20	-0.1395	0.0000	0.9902	-0.383 a* + 0.924 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: -14.30 -21.88 36.18

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:

51.82	0.0000	1.0000	0.0000
-------	--------	--------	--------

Anisotropy ratio: 0.854 [= (Emax - Emin) / Beq]
Fractional anisotropy: 0.434 [= sqrt(1.5 Sum_i (E_i - Beq)^2 / Sum_i E_i^2)]

Eigenvalues & eigenvectors of redundancy anisotropy tensor:

1.13	0.9576	0.0000	-0.2882	0.991 a* - 0.136 c*
0.71	0.0000	1.0000	0.0000	b*
0.43	0.2882	0.0000	0.9576	0.681 a* + 0.732 c*

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

2.36	0.9907	0.0000	-0.1360	0.997 a* - 0.083 c*
1.64	0.0000	1.0000	0.0000	b*
1.00	0.1360	0.0000	0.9907	0.385 a* + 0.923 c*

Eigenvalues & eigenvectors of weighted CC_{1/2} anisotropy tensor:

0.371	0.9829	0.0000	-0.1840	0.995 a* - 0.099 c*
0.286	0.0000	1.0000	0.0000	b*
0.184	0.1840	0.0000	0.9829	0.496 a* + 0.868 c*

Eigenvalues & eigenvectors of Z(weighted CC_{1/2}) anisotropy tensor:

61.15	0.9663	0.0000	-0.2575	0.992 a* - 0.125 c*
43.77	0.0000	1.0000	0.0000	b*
29.55	0.2575	0.0000	0.9663	0.634 a* + 0.773 c*

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

0.242	0.9893	0.0000	-0.1457	0.996 a* - 0.086 c*
0.178	0.0000	1.0000	0.0000	b*
0.111	0.1457	0.0000	0.9893	0.409 a* + 0.913 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						
1	Blue						
				Unobservable*			
				Observable*			
2	Red Pink:9	1	1.20	0.5000	45.00	0.184	0.0263
3	Orange	2	4.05	0.8935	137.07	0.534	0.0740
4	Yellow	3	9.67	0.9539	185.41	0.934	0.1754
5	Green	4	14.52	0.9642	213.01	1.148	0.3497
6	Cyan	5	18.85	0.9716	233.80	1.307	0.5862
7	Magenta	6	23.55	0.9791	262.10	1.619	0.8265
8	White	7	25.69	0.9829	279.67	1.999	0.9800

* 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: 6.45 [= 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:** $-\log P(\chi^2)$ ☒ Redundancy ☒ Mean $I/\sigma(I)$ ☒ Weighted $CC\frac{1}{2}$ ☐ $Z(wCC\frac{1}{2})$ ☐ **Experimental:** Kullback-Leibler divergence ☐ Cut-off surface ☒ Debye-Waller factor

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.