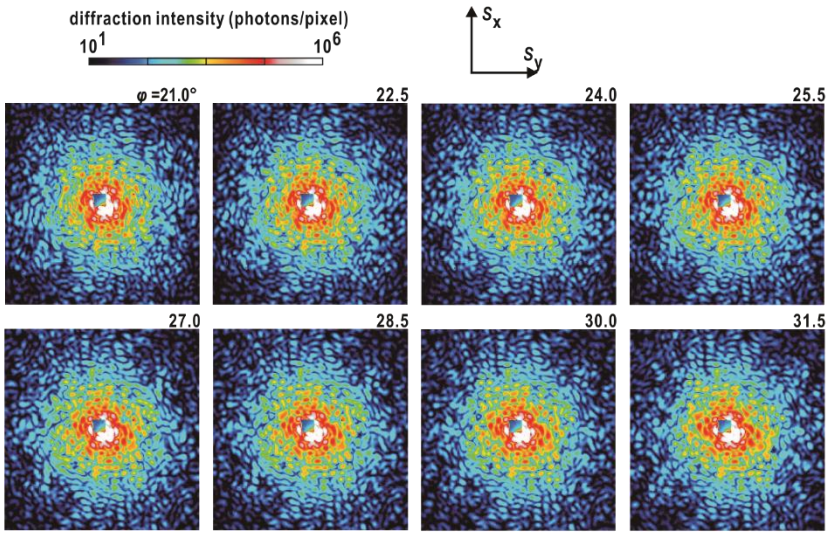
JOURNAL OF SYNCHROTRON RADIATION

Volume 25 (2018)

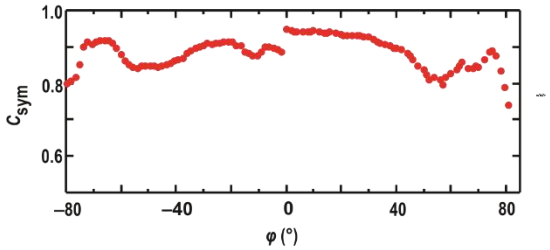
Supporting information for article:

Diffraction apparatus and procedure in tomography X-ray diffraction imaging for biological cells at cryogenic temperature using synchrotron X-ray radiation

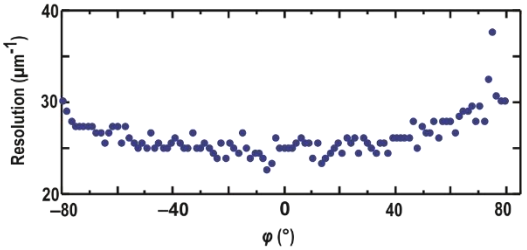
Amane Kobayashi, Yuki Takayama, Koji Okajima, Mao Oide, Takahiro Yamamoto, Yuki Sekiguchi, Tomotaka Oroguchi, Masayoshi Nakasako, Yoshiki Kohmura, Masaki Yamamoto, Takahiko Hoshi and Yasufumi Torizuka


diffraction intensity (photons/pixel)
10^1
10^6
S_x
S_y
φ =21.0°
22.5
24.0
25.5
27.0
28.5
30.0
31.5

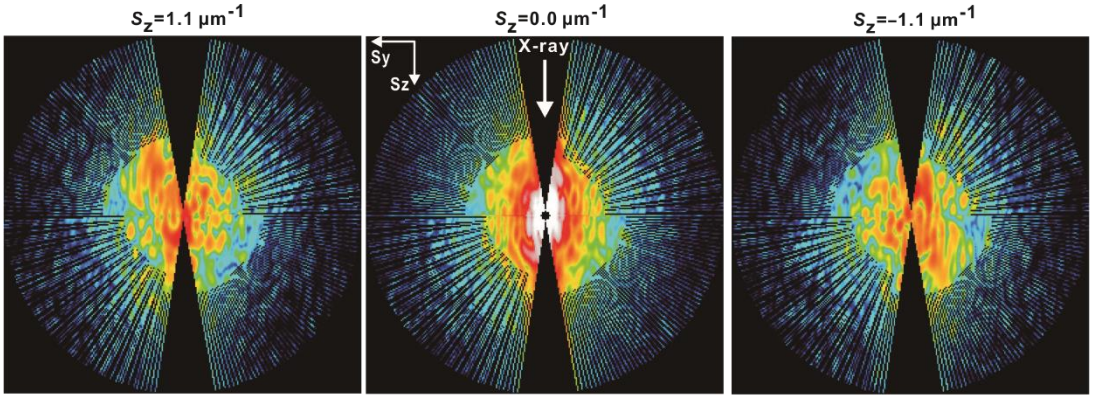
(a)


1.0
0.8
0.6
C_sym
–80
–40
0
40
80
φ (°)

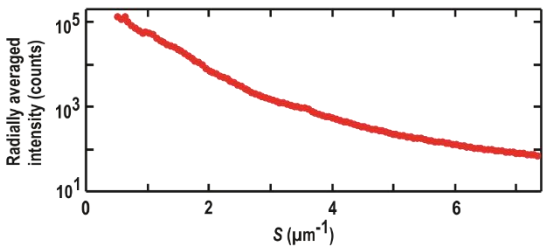
(b)


40
30
20
Resolution (μm^-1)
–80
–40
0
40
80
φ (°)

(c)


S_z=1.1 μm^-1
S_z=0.0 μm^-1
S_z=–1.1 μm^-1
Sy
Sz
X-ray

(d)


10^5
10^3
10^1
Radially averaged intensity (counts)
0
2
4
6
S (μm^-1)

(e)

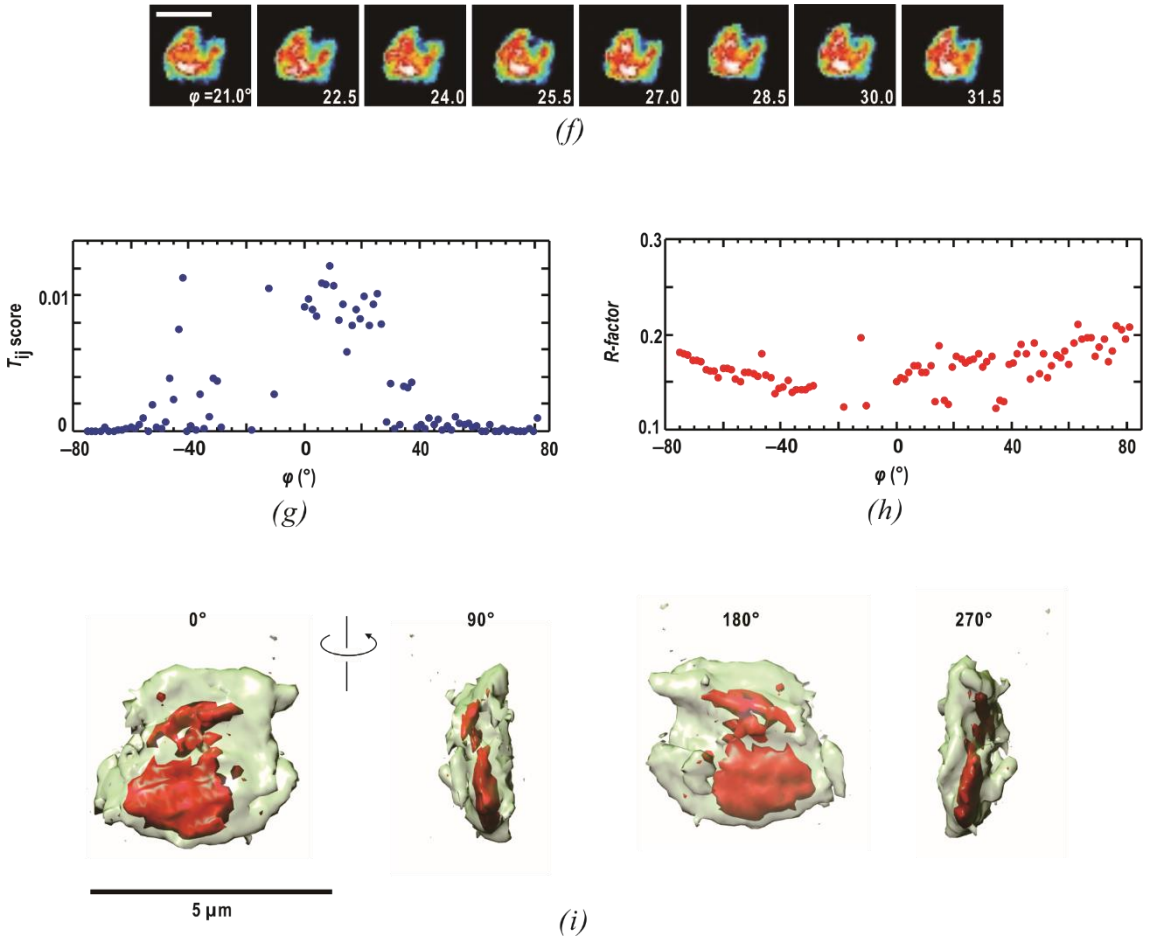


Figure S1 (a) Series of diffraction patterns from *S. cerevisiae* during a successive 1.5° rotation around φ=27°. The resolution at the edge is 6.31 μm^{-1}, corresponding to 158 nm in real space. The variation of C_{sym} values (b) and maximum resolution (c) plotted against the rotation angle. The C_{sym} values of most diffraction patterns were in the range of 0.8-0.95 except 70° < φ (Fig. 8(b)). Large speckle sizes tend to result in higher C_{sym} values, probably because of a high sampling ratio. The maximum resolution kept at 22-38 μm^{-1} implied little radiation damage to the cell. (d) The distribution of diffraction intensity in the S_y-S_z planes at S_x=1.1 (left panel), 0.0 (center), and –1.1 μm^{-1} (right). The resolution at the edge is 14.7 μm^{-1}. The reconstructed 3D distribution of the diffraction intensity was almost centrosymmetric. (e) The resolution-

dependent variation of radially averaged diffraction intensity. The radially averaged diffraction intensity reached a value of 10^5 in the small-angle region and decreased gradually to 10^2. (f) Projection electron density maps retrieved from the diffraction patterns in panel (a) at resolutions of 136 nm. The scale bar is 3 μm. The density maps in the successive series of rotation were similar to each other with respect to the sizes, shapes and internal structures. The variation of T_{ij} (g) and crystallographic *R*-factor (h) values of the PR map from each diffraction pattern are plotted against the rotation angle. The similarity scores T_{ij} were very small, and crystallographic *R*-factors were less than 0.2. These results suggested the success of PR calculations and the selection of the most probable maps. (i) Four views of 3D electron density maps of *S. cerevisiae* reconstructed by the 3D PR method. The maps are contoured to demonstrate the cell envelop and high density regions. The model is illustrated as Fig. 8(c) of the main text.