



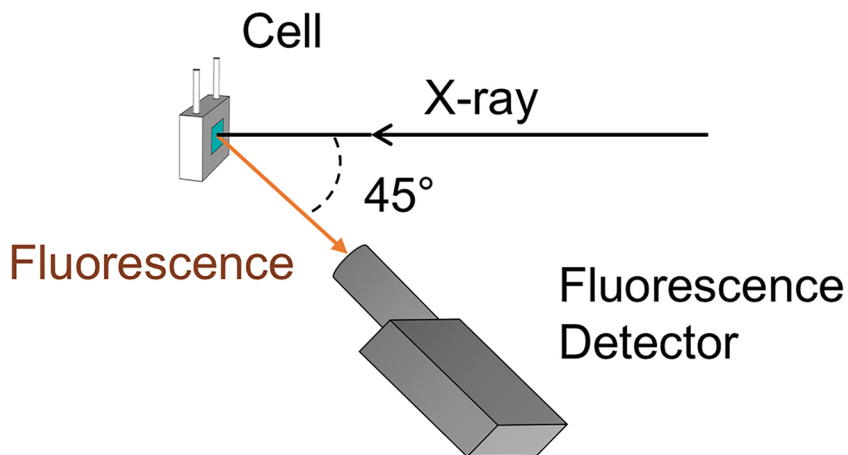
STRUCTURAL  
BIOLOGY

**Volume 78 (2022)**

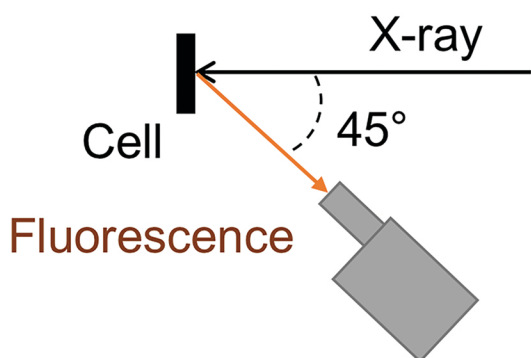
**Supporting information for article:**

***K*-edge anomalous SAXS for protein solution structure modeling**

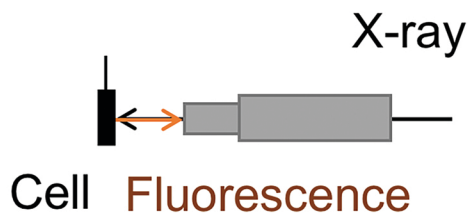
**Karman Virk, Kento Yonezawa, Komal Choukate, Lucky Singh, Nobutaka Shimizu and Barnali Chaudhuri**



Above view

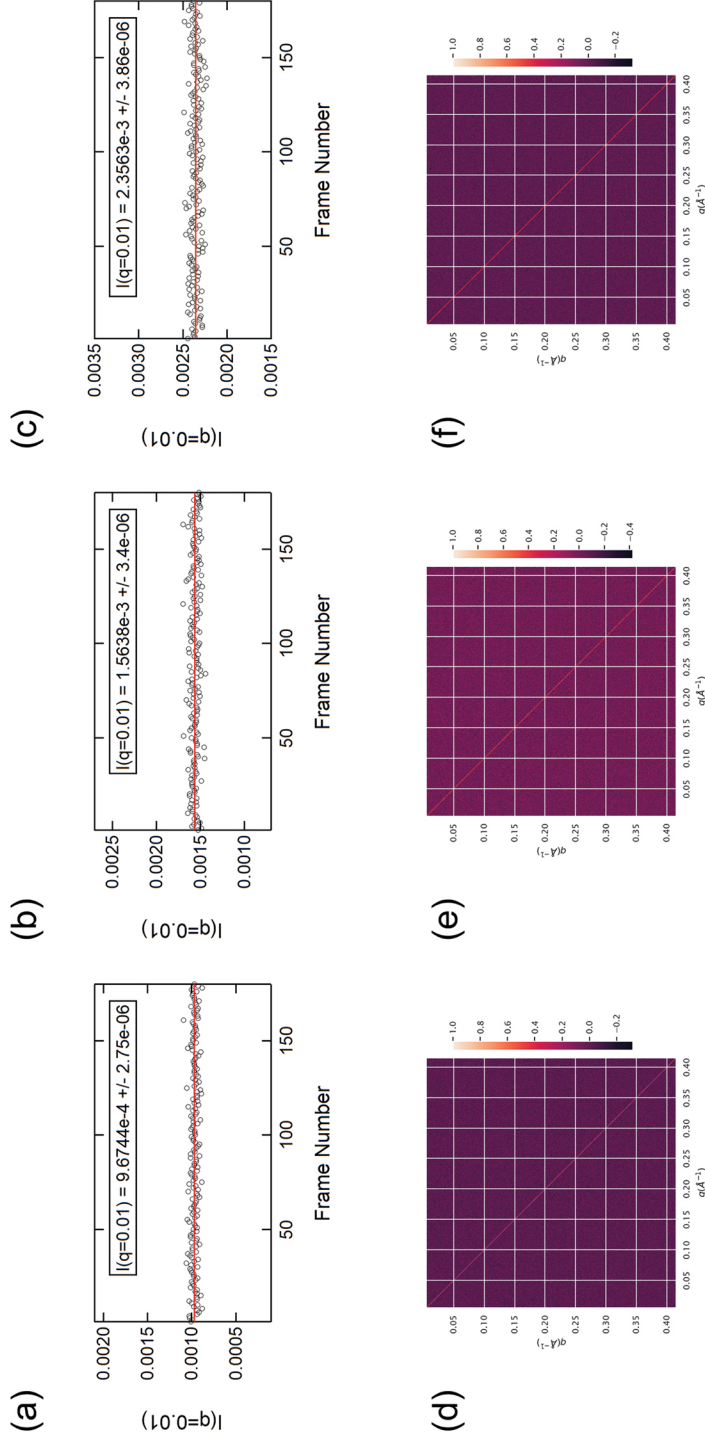


Side view



**Figure S1.** Schematic diagram of the experimental setup for XAS measurement at BL-15A2 beamline.

# Figure S2.



**Figure S2.** (a-c) The scattering intensities at  $q = 0.01 \text{ \AA}^{-1}$  during 180 measurements are shown for (a) buffer, (b) Myo10Chis and (c) Myo10ChisCu at 8989 eV. The red lines show the results of the linear approximations computed under the condition that the slope value is zero, and the values of the y-intercept and its standard deviation are noted in the graph. These calculations were carried out using Igor Pro (WaveMetrics). (d-f) Representative correlation maps obtained using the python module of CorMapAnalysis (Brooks-Bartlett et al., 2017) are shown for (d) buffer, (e) Myo10Chis and (f) Myo10ChisCu.

**Figure S3.** Plot of Guinier  $R_g$  in Å *versus* Energy (E in eV) for Myo10Chis and Myo10ChisCu datasets.

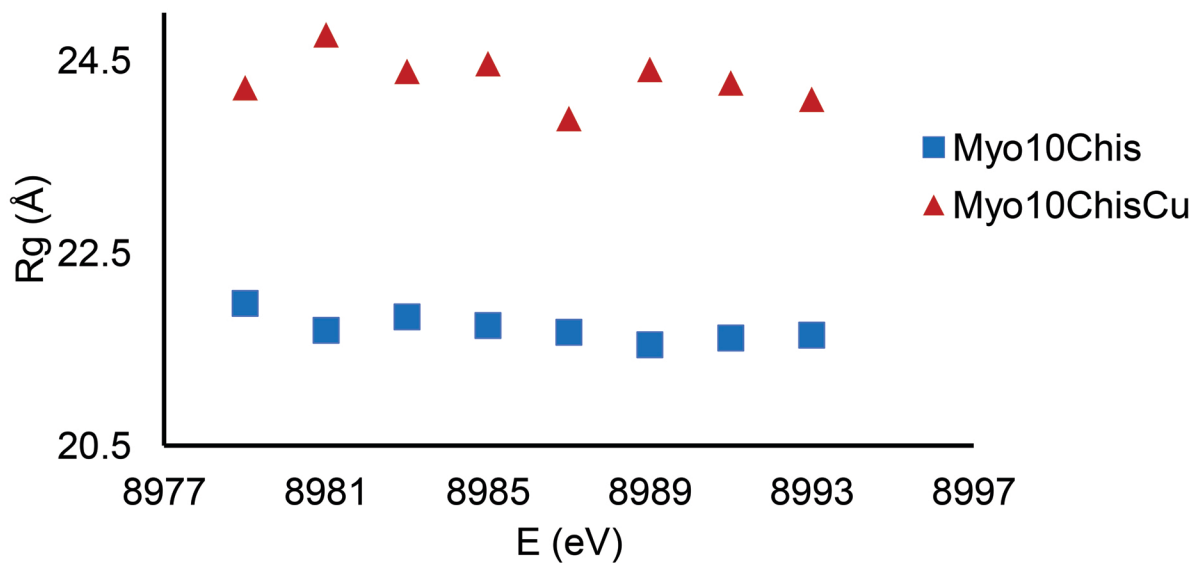
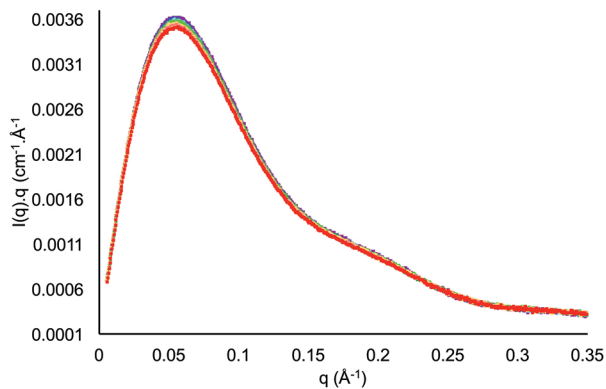
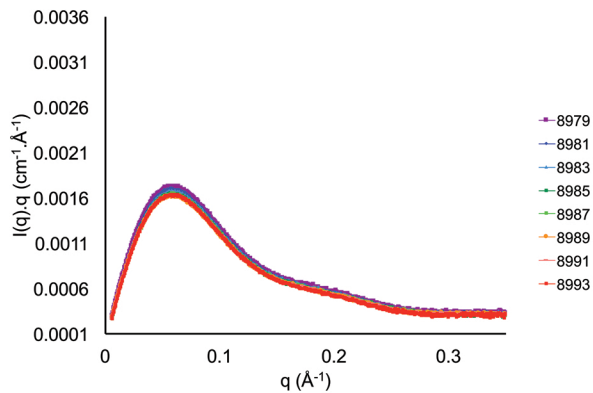




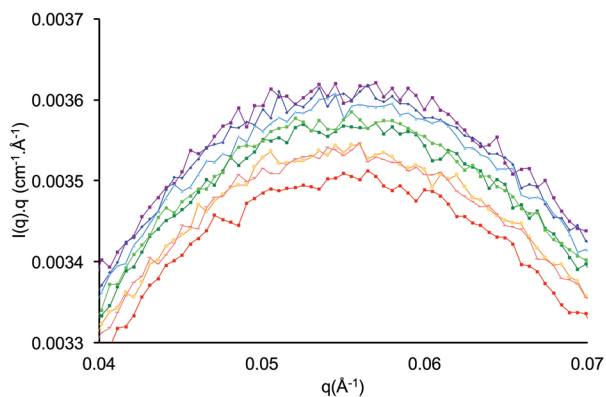
Figure S4.



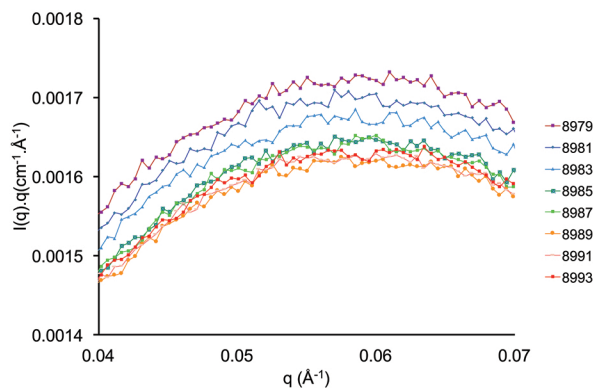
(a)



(b)



(c)



(d)

**Figure S4.** Holtzer plots ( $I(q).q$  versus  $q$ ,  $I$  in  $\text{cm}^{-1}$ ,  $q$  is  $\text{\AA}^{-1}$ ) of the (a-c) Myo10ChisCu (corrected for X-ray fluorescence) and (b-d) Myo10Chis SAXS datasets at various X-ray energies (8979, 8981, 8983, 8985, 8987, 8989, 8991, 8993 eVs) are shown.