Supplemental Information

1. Angular relations necessary to generate point group symmetry related projection directions for orthoaxial projections.

For C*n* symmetry, in order to generate necessary all symmetry-related projection directions from an orthoaxial projection direction $(\varphi, \theta = 90^{\circ}, \psi)$ within the unique range, the transformations are (Fig.S2):

1. for *n* even, unique range $\varphi \in [0,360/n)$: $\varphi_k = k \frac{360}{n} + \varphi$, $k = 0,...,\frac{n}{2} - 1$,

2. for *n* odd, unique range $\varphi \in [0,360/2n)$: $\varphi_k = k \frac{360}{n} + \varphi$, k = 0,...,n-1.

For D*n* symmetry, in order to generate necessary all symmetry-related projection directions from an orthoaxial projection direction $(\varphi, \theta = 90, \psi)$ within the unique range, the transformations are (Fig.S3):

1. for *n* even, unique range $\varphi \in [0,360/2n)$, we have k = 0,...,n-1, and

1.1. for *k* even,
$$\varphi_k = \frac{k}{2} \frac{360}{n} + \varphi$$

1.2. for *k* odd, additional change of in-plane rotation
 $\varphi_k = \left[\frac{k}{2}\right] \frac{360}{n} - \varphi + 180$, where [] means integer part of the division,
 $\psi_k = \psi + 180$

2. for *n* odd, unique range $\varphi \in [0,360/4n)$, we have k = 0,...,2n-1, and

2.1. for
$$k \mod 4 = 0$$
, $\varphi_k = \left[\frac{k}{4}\right] \frac{360}{n} + \varphi$,
2.2. for $k \mod 4 = 1$, $\begin{cases} \varphi_k = \left[\frac{k}{4}\right] \frac{360}{n} + \frac{360}{2n} + 180 - \varphi \\ \varphi_k = \psi + 180 \end{cases}$

2.3. for
$$k \mod 4 = 2$$
, $\varphi_k = \left\lfloor \frac{k}{4} \right\rfloor \frac{360}{n} + \frac{360}{2n} + 180 + \varphi$,

2.4. for
$$k \mod 4 = 3$$
,
$$\begin{cases} \varphi_k = \left[\frac{k}{4}\right] \frac{360}{n} + 2\frac{360}{2n} - \varphi \\ \psi_k = \psi + 180 \end{cases}$$

As can be seen from the above equations, in order to generate all necessary orthoaxial projections given a subset in unique range, we need to consider three operations on projection images: mirror, rotation by 180°, and combined mirror and rotation by 180°. Based on simple representations of four possible orientations (Fig.S1), we can illustrate the equations defining relations between orthoaxial projections using simple schematics (Figs.S2 and S3).



Figure S1: Overview of all four possible orientations of an orthoaxial projection within the unique range: (A) the original projection, (B) mirrored version of the original projection, (C) the 180° in-plane rotated original projection, and (D) mirrored version of the 180° in-plane rotated projection.



Figure S2: Schematic diagram of relations between orthoaxial projections within the full angular range ($\varphi \in [0,360^{\circ})$) for (A) C1 symmetry, (B) C3 symmetry, and (C) C4 symmetry. The blue arc represents the unique angular range. The progression of φ angle within the unique range is illustrated by three different-color arrows. Arrows outside the unique range with same color denote projections related to the same projection of the unique range.



Figure S3: Schematic diagram of relations between orthoaxial projections within the full angular range ($\varphi \in [0,360^{\circ})$) for (A) D1 symmetry, (B) D3 symmetry, and (C) D4 symmetry. The blue arc represents the unique angular range. The progression of φ angle within the unique range is illustrated by three different-color arrows. Arrows outside the unique range with same color denote projections related to the same projection of the unique range.

2. A Python program that computes pixel adjustment factor given original pixel

size, rise, and segment length:

#!/usr/bin/env python

def match pixel rise(dz, px, nz, rele = 0.1): # find pixel size closest to the given one (px) # such that rise (dz) is approximately equal to integer number of pixels # Input: # dz - axial rise [Angstrom] # px - pixel size [Angstrom] # nz - z length of the segment [pixel] rele - relative error of the approximation # # Output: # q - pixel size adjustment factor # error - relative error of resulting approximation $dnz = nz^*px$ # odd number of full disks in the segment $ndisk = 2^{((int(dnz/dz)-1)/2)} + 1$ # However, I believe we should only use half of them, # because error increase counting from the center of the volume ndisk = (int(dnz/dz)-1)/2q = 1.0 for i in xrange(900000): q = 1.0 - 0.000001*i error = ((int(ndisk*dz/q/px) - ndisk*dz/q/px)/px)**2 if(error < rele): return g,error return -1.0,-1.0 # execute program dz = 27.6 px = 1.31nz = 220 o = match_pixel_rise(dz, px, nz, 0.001) print o # The resampling is done using function resample of SPARX system:

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\#vn = resample(vo, 1.0/o[0])
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