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Supporting information for article:

Refining perovskite structures to pair distribution function data using collective Glazer modes as a basis

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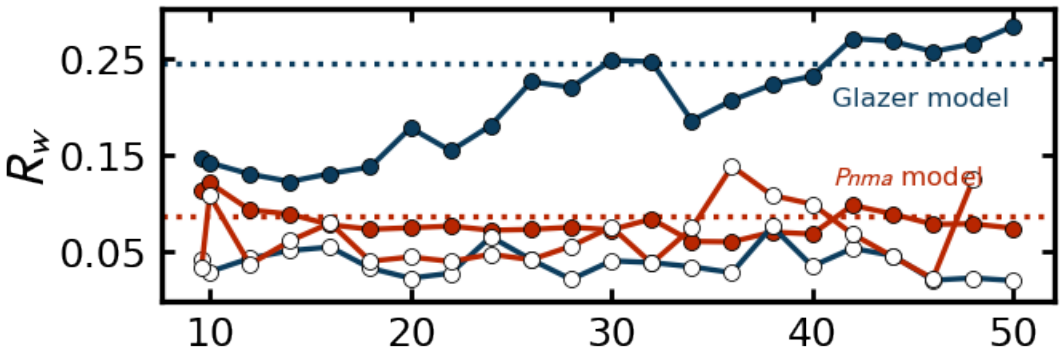

Figure S1: Comparison of the fit residual R_w from boxcar fits with the space group model (blue) and the Glazer model (red). The closed circles are fits of measured PDF data of $CaTiO_3$ at 200 K while the open circles are fits to simulated PDF of $CaTiO_3$. The simulated data were calculated from a constructed 2x2x2 unit cell with tilt system $\alpha^+ \beta^- \beta^-$, where tilt angles $\alpha = 9^\circ$ and $\beta = 10^\circ$. The Ca displacements and the isotropic thermal displacement parameters (U_{iso}) for each element were chosen according to fits with the space group model of the measured $CaTiO_3$ at 200 K.