Structure factors $|F|^2 = \sum_i \delta_i f_i e^{i\mathbf{q}\cdot\mathbf{a_i}}$ are calculated for PMN. The elastic structure factors are related to the Bragg peak intensity as well as diffuse scatterings coming from a uniform shift ($\delta_{Pb} = \delta_{Mg,Nb} = \delta_O = 1.0$). The inelastic structure factors are related to intensity from a soft-mode with center of mass at zero. For the inelastic intensity, another parameter $S = S2/S1$, the ratio of the S2-Last mode and the S1-Slater mode is introduced. The atomic displacements for the inelastic structure factors are calculated as,
$\delta_P b = -S(M_{Mg,Nb} + 3M_O)/M_{Pb}$
$\delta_{Mg,Nb} = -3M_O/M_{Mg,Nb} + S$
$\delta_O = 1 + S$,
and then normalized to $\delta_O = 1.0$.

We only show structure factors from (100), (110) and (200). (300) has the same structure factor $|F|^2$ as (100), (220) the same as (200). Their intensities only differ due to the $\sin 2\theta$ factor.

Reflection	Elastic	Inelastic		
		S=0	S=1	S=2
100	8.39	1.83	90.30	149.3
110	101.8	105.1	55.6	42.6
200	1109	167.9	248.2	278.4

Table 1: Neutron structure factors for PMN

Reflection	Elastic	Inelastic		
		S=0	S=1	S=2
100	1820	181.5	1316	2796
110	11095	868.6	698.4	645.8
200	18860	6.39	31.0	43.4

Table 2: Xray structure factors for PMN

Here we also show structure factors based on Vakhrushev's results ($\delta_{Pb} = 1.0, \delta_{Mg,Nb} = 0.18, \delta_O = -0.64$),

Reflection	Neutron Struc. Fac.	X-ray Struc. Fac.
100	142	6638
110	204	8604
200	0.33	5224

Table 3: Structure factors, calculated based on atomic shifts from Vakhrushev for PMN