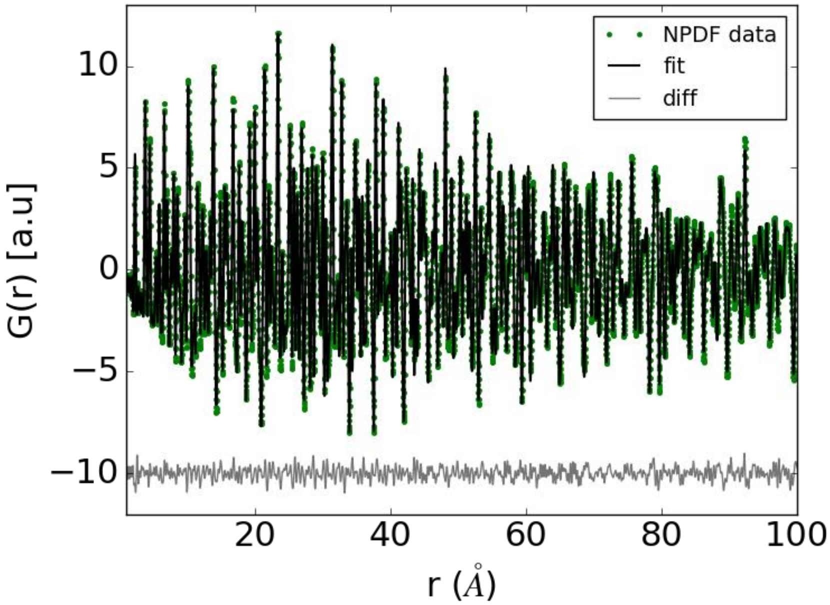
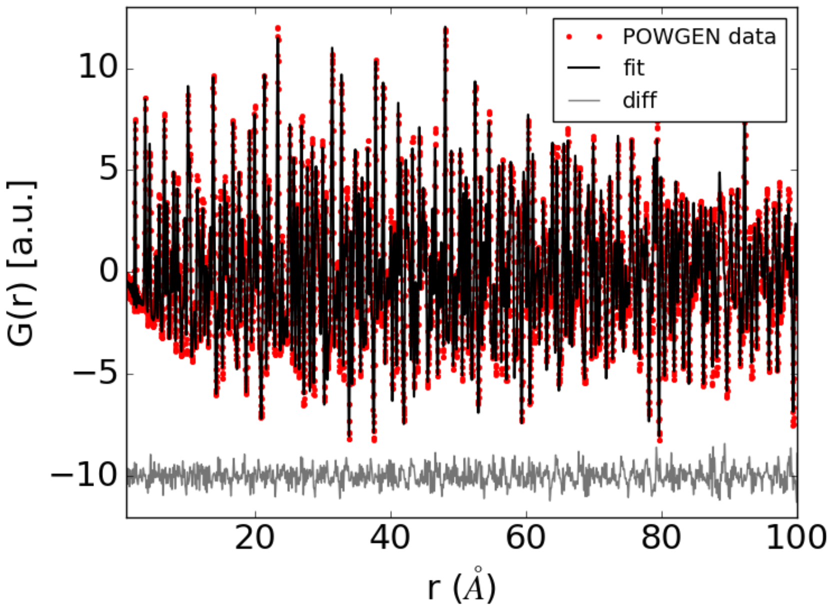
Comparison of fits in PDFgui to Si-standard on three neutron TOF diffractometers

These three datasets, along with the simulated patterns used in the manuscript, are available upon request from the authors.

NPDF - PDFgui fit : r_{min} = 1.0 Å, r_{max} = 100.0 Å, Δr = 0.02 Å



POWGEN - PDFgui fit : r_{min} = 1.0 Å, r_{max} = 100.0 Å, Δr = 0.02 Å



NOMAD - PDFgui fit : r_{min} = 1.0 Å, r_{max} = 100.0 Å, Δr = 0.02 Å

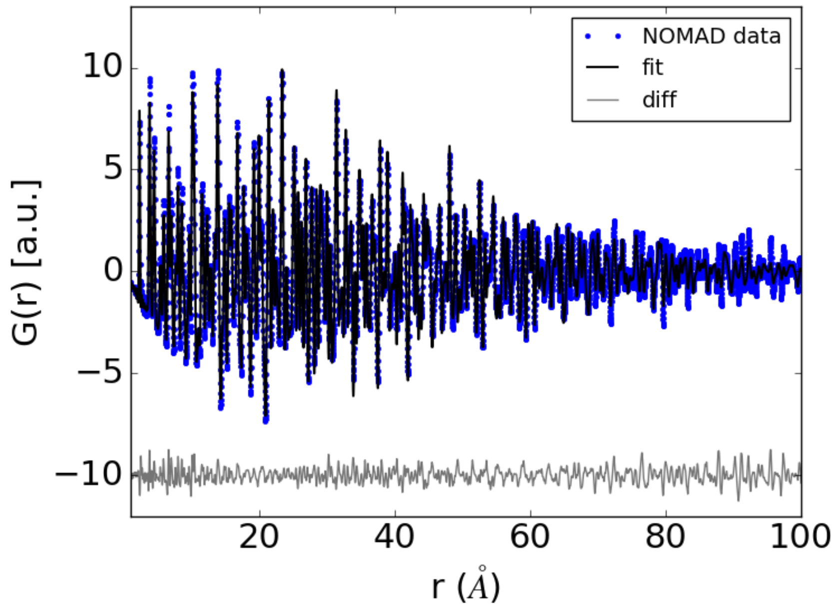


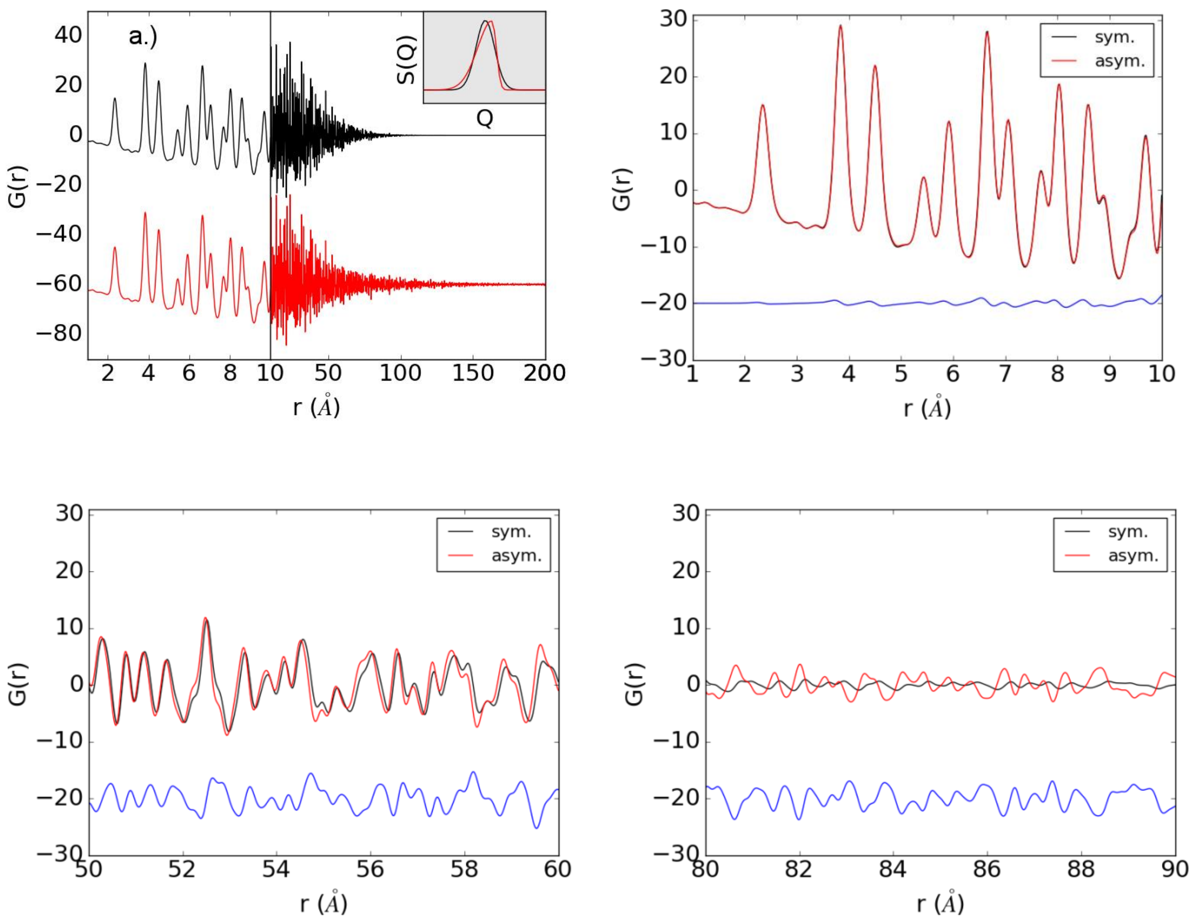
Table of refined values from PDFgui fits

Parameter	NPDF	POWGEN	NOMAD
a (Å)	5.43391	5.43033	5.43185
U_{iso} (Å^2)	0.005763	0.005388	0.007976
Scale	0.703675	0.727372	1.274774
Delta2	3.860761	4.172002	4.259381
Q_{damp}	0.004979	0.007322	0.021206
Q_{broad}	0.015247	0.006932	0.010516
R_{wp}	0.098172	0.122800	0.158530

These three fits were performed using standard data fitting procedures with PDFgui. They are presented here as a comparison and general indications of how the different instrument characteristics are accommodated in fitting approaches employed by PDFgui.

Comparison of PDFs due to symmetric vs. asymmetric peaks

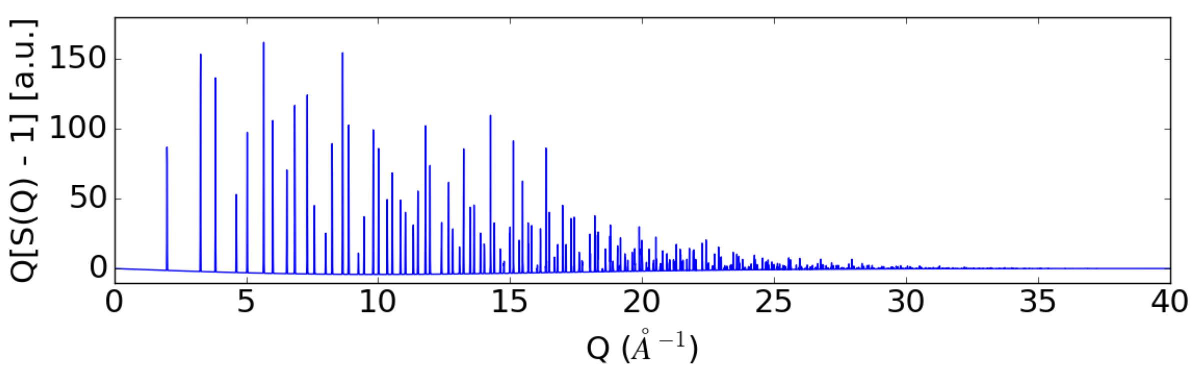
These PDFs are those calculated from the asymmetric (red) and symmetric (black) Gaussian peak shapes, as discussed in section 2.3 (Fig. 5) of the manuscript. The difference between them (symmetric – asymmetric) is offset below each plot. The described apparent shifting of the lattice constant is clearly seen in the mid- and high-r plots, although the difference in damping factor between the two is significant by high-r. The initial plot from Fig. 5 a) is also presented for comparison.

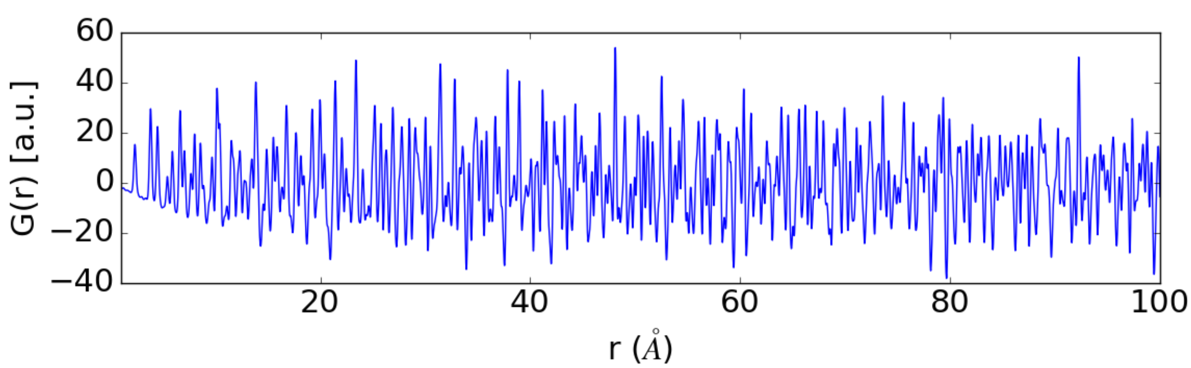


Method of simulating Si-dataset for comparisons in manuscript

For each of these examples, we utilize a hybrid simulated/measured dataset of NIST standard Si (SRM 640). This initial data was gathered on NOMAD in 6 mm vanadium cans, and measured for 6 hours to ensure optimal data quality. Rietveld refinements were performed using TOPAS with data from the four highest resolution banks on NOMAD (centered at 31, 67, 122, and 154 degrees), where the lattice constant of the material was fixed to the published value. Using the as-fit d-spacing, the model peaks were then replaced with narrow Gaussian peaks, and extended to beyond the d-spacing measurable by the high-resolution bank (as this bank natively has a limited lower bandwidth of Q_{min} = 6 Å^{-1}). The as fit background function was also subtracted. The d-dependence of the peak intensity was fixed at d^4.

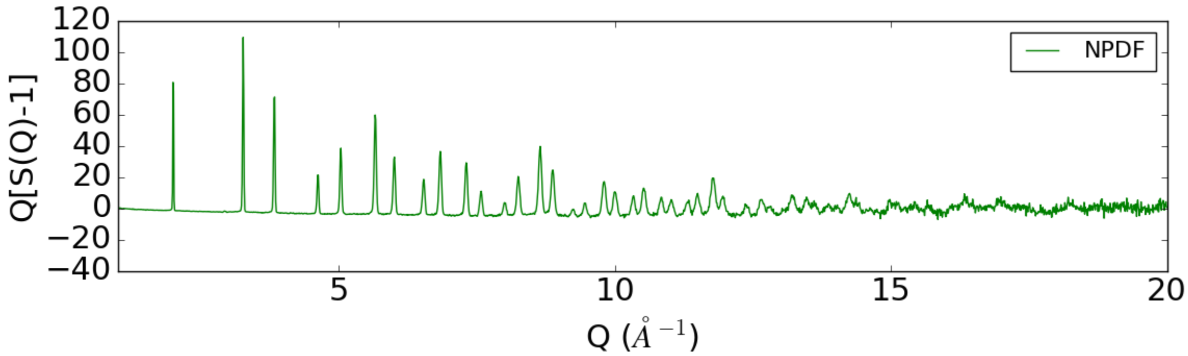
To generate a synthetic total scattering structure factor, [S(Q)-1], a Debye-Waller factor is subtracted from the data, which was fit to most accurately reproduce the effect seen in the as-measured [S(Q)-1] in the NOMAD data. A sine-transform of Q[S(Q) – 1] thus results in the simulated ideal G(r). A fit of this ideal G(r) data to the known Si structure with PDFgui was found to reproduce high-quality results from 1 to 80 Angstroms (Rw < 3%). The results of that fit are shown in below. We use this synthetic data as a starting point for our simulations of the various resolution effects on the overall PDF quality. This idealized Q[S(Q)-1] and PDF are plotted below.

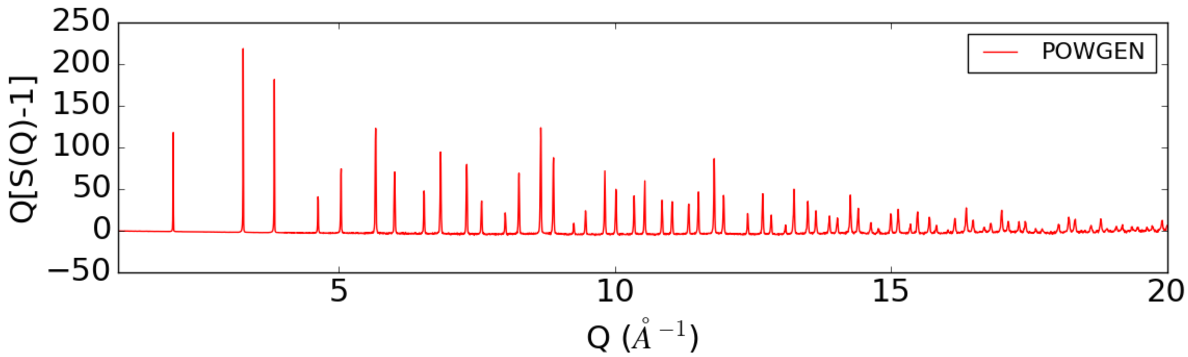


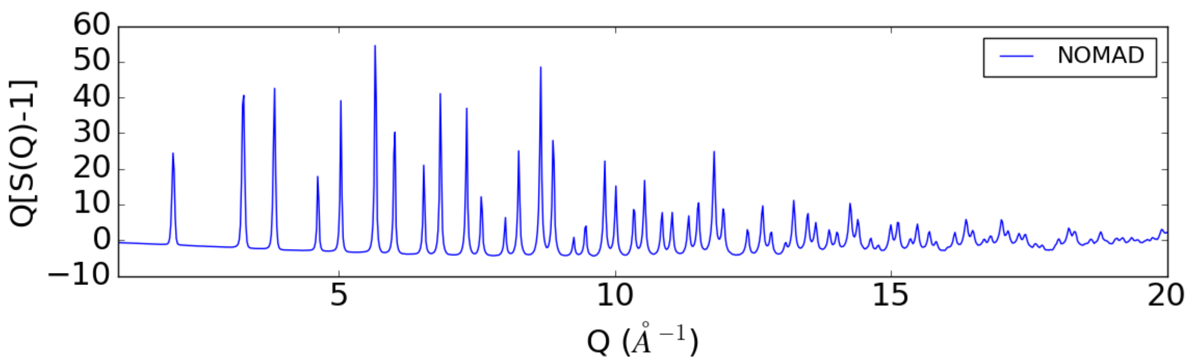


<u>**As-reduced datasets from three neutron TOF diffractometers**</u>

The as-reduced datasets, using standard data reduction procedures of each beamline, is shown below. Note these procedures can differ, and produce reciprocal space data with different intensity factors, though all have been normalized to the measured scattering from a vanadium rod. While the details of those differences are beyond the scope of this manuscript, the effect on the resultant PDF analyis is minimal via small box modeling approaches, where a scale factor is regularly employed in the real-space refinement. Full data normalization procedures (including factors such as absorption, density, packing fraction, etc.) are much more critical to RMC-style data analysis.







At the time of writing, new data reduction procedures are actively being developed on NOMAD and POWGEN. Readers interested in the measured standards are encouraged to contact the instrument teams to receive the latest standard datasets for comparison, as well as the details of reduction methods currently employed on each beamline.