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Supporting information for article:

**Why Direct and Post-refinement Determinations of Absolute
Structure May Give Different Results**

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S1. Excel spreadsheet for all six procedures on all 28 materials

There are six rows of data for each structure (Table 5). The first pair of rows (A&B) give the absolute structure analysis results for the full matrix refinement with SHELX weights. The second pair of rows (C&D) is the same information when only the overall scale and Flack(x) parameters were further refined. In every case rows A&B are almost identical to rows C&D, indicating that for a fully refined structure there is little correlation between the structural parameters and the absolute structure parameters. The last pair of rows (E&F) were obtained when only the scale and Flack(x) parameter were refined using weights computed from unmodified intensity variances. Within each pair of rows, the first row contains post-refinement values using weights computed from the intensity variances, the second row contains post-refinement values using weights computed from the weights used in the main least squares.

Table S1 Key to the layout of information in S1.

Row id	Paper id	Structure Id	Refinement flag	Refinement conditions	Post refinement	Post-refinement conditions
A	HDF	sf3166	Full	Full matrix with SHELX weights	SIG	Observational weights
B	HDF	sf3166	Full		LSQ	Main refinement weights
C	HDF	sf3166	Scheme	Scale and Flack only, with SHELX weights	SIG	Observational weights
D	HDF	sf3166	Scheme		LSQ	Main refinement weights
E	HDF	sf3166	Counting	Scale and Flack only, with counting statistic weights	SIG	Observational weights
F	HDF	sf3166	Counting		LSQ	Main refinement weights

S2. Excel spreadsheet for the statistically weighted post-refinement analyses of all 28 materials.**Table S2** Key to the layout of information in S2

Paper id	Structure Id	Refinement flag	Refinement conditions	Post refinement	Post-refinement conditions
HDF	YIFZAP	Scheme	Scale and Flack only, with SHELX weights	SIG	Observational weights