Appendix A. Criteria and filters used in CSD searches

The following criteria were used when searching the CSD for the crystal structures used to generate Figures 2-5: 3D coordinates determined = TRUE; *R*-factor = ANY; Not disordered = TRUE; No errors = TRUE; Only organics = TRUE; Z' = 1. Replicate structures, or structures reported at multiple temperatures or pressures were not eliminated from the search results. Structures with Z' < 1 were excluded as not being representative of pharmaceuticals. Excluding Z' > 1 structures from the search eliminates only *ca*. 10% of powder structures but simplifies calculation of degrees of freedom.

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