Towards solution and refinement of organic crystal structures by fitting to the atomic pair distribution function

Dragica Prill, Pavol Juhás, Simon J. L. Billinge and Martin U. Schmidt
Details of the CSD search for paracetamol

Search fragment:

- Q – either N or C atom
- x – either 2 or 3
- a – atom not involved in a ring

All disordered structures were excluded.

Fig. S1: Distribution of the torsion angle $\tau_1$ between the phenyl ring and the amide group.
Fig. S2: Distribution of the torsion angle $\tau_2$ between the PhNH and the COCH$_3$ group.