FOUNDATIONS
ADVANCES

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Supporting information for article:

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

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Supplementary Material

for the article:

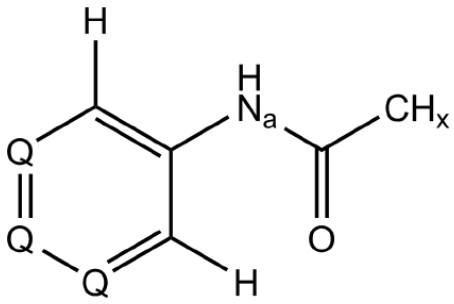
"Towards solution and refinement of organic crystal structures by fitting to the atomic pair distribution function"

by

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.

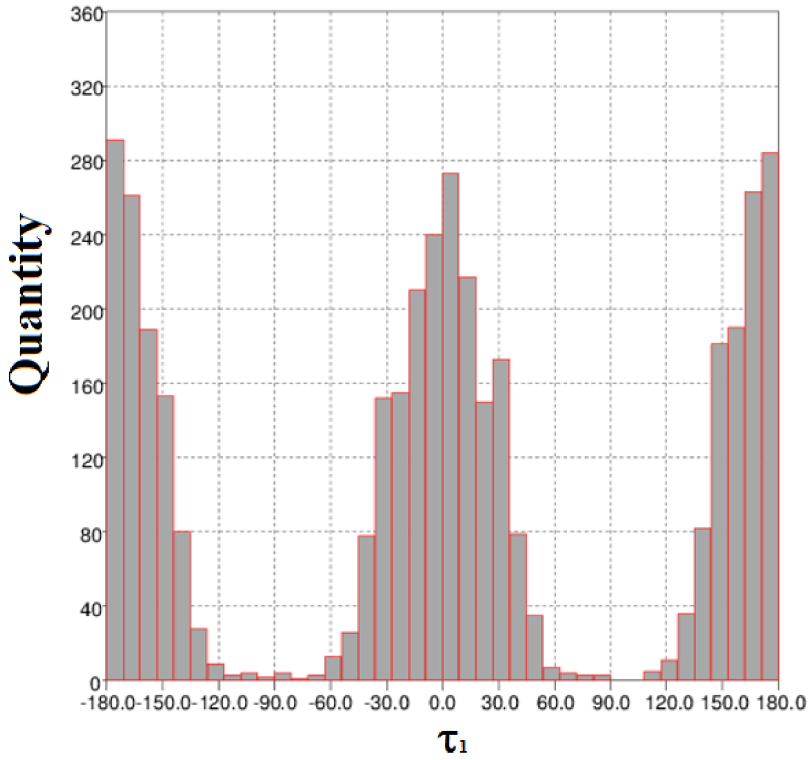


Fig. S1: Distribution of the torsion angle τ_1 between the phenyl ring and the amide group.

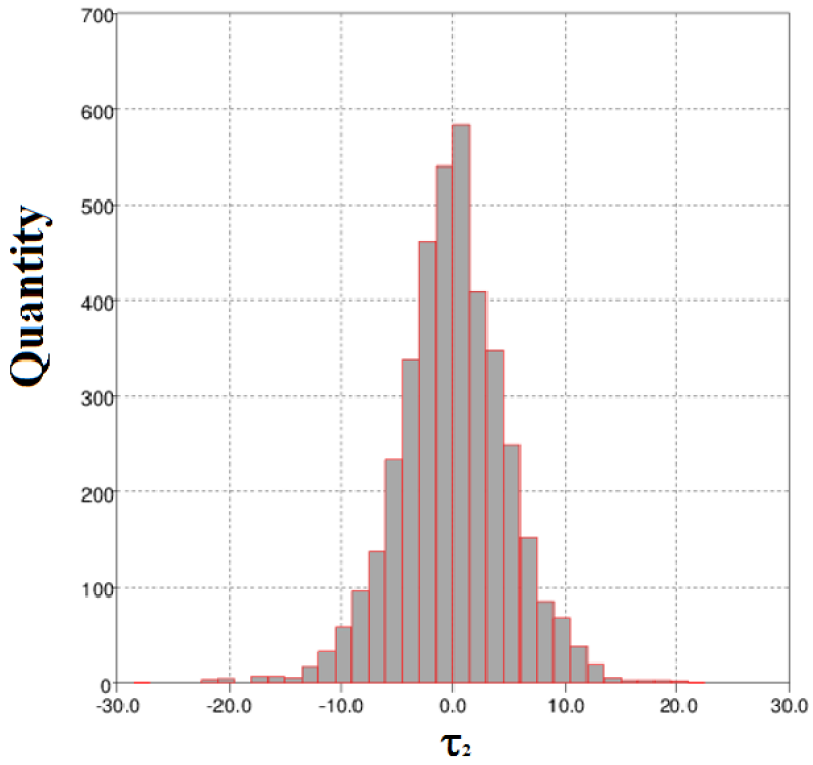


Fig. S2: Distribution of the torsion angle τ_2 between the PhNH and the $COCH_3$ group.