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Supporting information for article:

A chiral diamine: practical implications of a three stereoisomer cocrystallization

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S1. Results of SCD searches

All searches were performed against the CSD v5.381 (Groom *et al.*, 2016) using the CSD Python API v1.3. The Python scripts used to perform the searches are attached as part of the supplementary material of this manuscript. First, the CSD was filtered to find single component structures with at least one stereogenic center. For each structure in this set, all stereocentres in the unit cell were identified and assessed on a per molecule basis. The list of stereocentres thus identified was reduced to remove any duplicates so that, for example, "*R, R*; *R, R*; *S, S*" becomes "*R, R*; *S, S*". These patterns were then compared to predefined sets to identify the entries in the CSD that matched the desired criteria for subsequent analysis.

The subsets of individual structures with two anomeric carbon atoms were identified as follows:

- Those that contained the "*R*, *R*", "*S*, *S*" and "*R*, *S*" enantiomers in the crystal (rr_rs_ss_match.gcd)
- Those containing only the "*R, S*" isomer in the crystal (rs_match.gcd)
- Those containing only the "*R*, *R*" or "*S*, *S*" enantiomers in the crystal (rr_match.gcd or ss_match.gcd respectively)
- Those containing both the "*R*, *R*" and "*S*, *S*", but not the "*R, S*" enantiomer in the crystal (rr_ss_match.gcd)

The results of the CSD search for the high-quality CHN structures are presented in file CHN_best_r-factor.gcd.