Table S1. Crystal Data for DHCBZ:AcOH.

DHCBZ : AcOH			
Empirical Formula	$C_{17}H_{18}N_2O_3$	**Z**	4
Formula weight	298.33	***Radiation type***	Mo-K α
Space Group	*Monoclinic, P2₁/c*	**D_c (Mg/m^3)**	1.300
a (Å)	18.7201(6)	**λ (Å)**	0.71073
b (Å)	15.4255(4)	**θ_{max} (º)**	27.48
c (Å)	5.2995(10)	**Reflections Collected**	*12860*
β (º)	95.1740(10)	**Unique reflections**	3455 (R_{int} = 0.0533)
V (Å^3)	1524.08(7)	**Final R indices for 204 parameters [$I > 2\sigma(I)$]**	R_1 = 0.0429, wR_2 = 0.1032
T (K)	120(2)	**R indices all data**	R_1 = 0.0578, wR_2 = 0.1119

Lattice energy minimizations were performed in an identical way to those reported in our previous study of pure carbamazepine crystal structures (reference 15), i.e. using DFT optimized molecular structures, a distributed multipole analysis of a DFT calculated wavefunction for the intermolecular electrostatic potential and an *exp-6* intermolecular model potential using the W99 model potential parameters. Molecules were treated as rigid except for the pyramidalization of the amide group, whose flexibility was considered using the method described in reference 15. All lattice energy minimizations were performed using the DMAREL crystal structure modeling program.

Table S2. Space groups, calculated densities and energies and classification of the hydrogen bond and packing motifs (as in reference 15) for the ten most stable predicted structures for CBZ:AcOH and DHCBZ:AcOH.

		CIF file frame	**Space Group**	**DMA density**	**Total DMA energy**	**HBond Motif**	**Packing Motif**
CBZ:AcOH	Matches Experimental	***1***	***$P2_1/c$***	***1.295***	***-175.75***	***heterodimer***	***π-π stacking***
		2	$P2_12_12_1$	1.264	-174.59	heterodimer	Other
		3	$P2_1/c$	1.268	-173.01	heterodimer	Other
		4	$\bar{P}1$	1.283	-171.34	heterodimer	π-π stacking
		5	$\bar{P}1$	1.272	-171.13	homodimer	Sandwich-Herringbone
		6	$P2_1/c$	1.283	-171.11	heterodimer	Other
		7	$P2_1/c$	1.254	-170.89	heterodimer	Other
		8	$P2_1$	1.267	-170.79	heterodimer	Other
		9	$P2_1/c$	1.267	-170.27	heterodimer	π-π stacking
		10	$C2/c$	1.300	-169.95	heterodimer	π-π stacking
DHCBZ:AcOH	Matches Experimental	1	$\bar{P}1$	1.274	-173.70	heterodimer	π-π stacking
		2	$P2_1/c$	1.312	-173.33	AcOH-dimer DHCBZ-none	Sandwich-Herringbone
		3	***$P2_1/c$***	***1.241***	***-171.75***	***heterodimer***	***π-π stacking***
		4	$P2_1/c$	1.249	-171.70	heterodimer	π-π stacking
		5	$\bar{P}1$	1.303	-171.70	AcOH-dimer DHCBZ-none	Sandwich-Herringbone

		6	$\bar{P}1$	1.248	-170.50	homodimer	Other
		7	$\bar{P}1$	1.248	-170.31	homodimer	Sandwich-Herringbone
		8	$\bar{P}1$	1.250	-170.29	heterodimer	Sandwich-Herringbone
		9	$P2_1/c$	1.304	-169.94	AcOH-dimer DHCBZ-none	Sandwich-Herringbone
		10	$P2_1/c$	1.271	-168.80	heterodimer	Sandwich-Herringbone

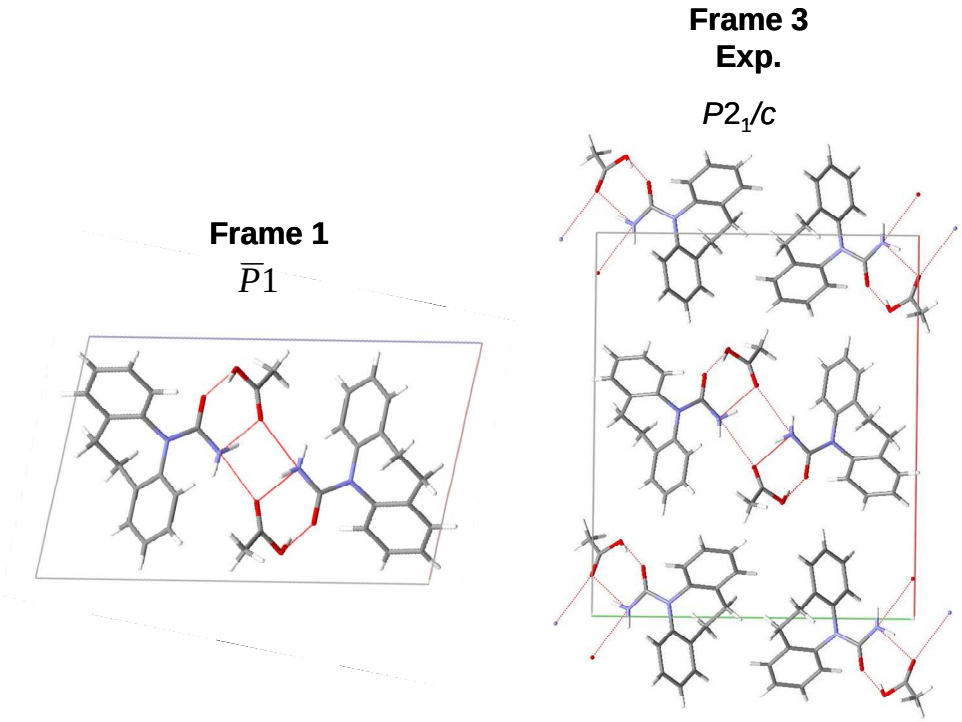

Figure S1. Representation of the unit cells for the most stable predicted (left, $\bar{P}1$) and the observed (right, $P2_1/c$) DHCBZ:AcOH crystal structures.

Reference 1 with a complete list of authors:

Day, G. M.; Motherwell, S.; Ammon, H. L.; Boerrigter, S. X. M.; Della Valle, R. G.; Venuti, E.; Dzyabchenko, A.; Dunitz, J. D.; Schweizer, B.; van Eijck, B. P.; Facelli, J. C.; Bazterra, V. E.; Ferraro, M. B.; Hofmann, D. W. M.; Leusen, F. J. J.; Liang, C.; Pantelides, C. C.; Karamertzanis, P. G.; Price, S. L.; Lewis, T. C.; Nowell, H.; Torrisi, A.; Scheraga, H.; Arnautova, Y. A.; Schmidt, M. U.; Verwer, P. *Acta Crystallogr. Sect. B: Struct. Sci.* **2005**, *61*, 511-527.