Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Disorder in Molecular Crystals Justified with the Help of Statistical Mechanics: A Case of Two Enantiomer Solid Solutions

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Table S1. Lattice energy (kJ/mol) breakdown of compound **1** canonical ensemble local structures (interaction energy half-sum of each of *Z* molecules (A, B, C, D) and molecules within an 11 Å sphere around its centroid).

Struct.	**A**	**B**	**C**	**D**	**Average**
#0	-151.0	-151.0	-151.0	-151.0	**-151.0**
#1	-150.2	-146.3	-142.0	-151.2	**-147.4**
#5	-150.5	-147.6	-147.6	-150.5	**-149.0**
#6	-141.3	-147.0	-141.2	-147.0	**-144.1**
#7	-146.0	-145.9	-142.7	-142.9	**-144.4**
#11	-141.6	-148.3	-146.7	-146.2	**-145.7**
#15	-146.9	-146.9	-146.9	-146.9	**-146.9**

Table S2. Lattice energy (kJ/mol) breakdown of compound **1** and **2** canonical ensemble local structures (interaction energy half-sum of each of *Z* molecules (A, B, C, D) and molecules within an 25 Å sphere around its centroid).

Struct.	**A**	**B**	**C**	**D**	**Average**
1					
#0	-154.5	-154.5	-154.5	-154.5	**-154.5**
#1	-154.3	-149.8	-145.8	-154.9	**-151.2**
#5	-154.9	-151.6	-151.5	-155.0	**-153.2**
2					
#0	-125.7	-126.4	-125.7	-126.4	**-126.0**
#1	-125.3	-122.7	-125.3	-122.7	**-124.0**
#2	-128.6	-125.4	-124.5	-123.8	**-125.6**