A modulated cocrystal: 
$N'-(\text{propan-2-ylidene})\text{nicotinohydrazide and sebacic acid}$

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Trying to cocrystallise nicotinic acid hydrazide ($n\text{iazid}$) with sebacic acid from an acetone solution, resulted in a reaction of the $n\text{iazid}$ with the solvent. Cocrystals were formed, which contain molecules of $N'-(\text{propan-2-ylidene})\text{nicotinohydrazide (p-niazid)}$ and sebacic acid [1]. These cocrystals exhibit an incommensurately modulated structure. Structural analysis was performed using single-crystal X-ray diffraction data, collected at 173 K. After solution and refinement of the average structure (which includes disorder of the sebacic acid molecule) the modulated structure was refined using the (3+1)-dimensional superspace approach [2]. The structure belongs to the planar monoclinic crystal system ($a=5.07$, $b=44.51$, $c=6.40\text{Å}$, $\beta=94.6^\circ$, $q=\langle-0.08, \ 0, \ 0.26\rangle$) and the superspace group was determined to be $P2_1/n(\alpha\ 0\ \gamma)00$.

Harmonic modulation functions of first order were successively introduced for all atom positions, but refined for non-hydrogen atoms only. The positions and modulation functions of the hydrogen atoms were fixed due to geometrical constraints. The final refinement included harmonic modulation waves for coordinates and ADPs for all non-hydrogen atoms. The $p$-niazid molecule, as well as the carboxylic groups of the sebacic acid are not much affected by the modulation, whereas the atoms of the hydrocarbon chain of the acid show a strong coordinated displacive modulation. The plane of the C-C bonds exhibits a rotation of up to $45^\circ$ about the centre line of the ribbon. The crystal structure shows slabs packed with sebacic acid. These layers are oriented perpendicular to $b$ and the sebacic acid molecules are tilted about $54^\circ$ against $b$. We assume that weak intermolecular interactions within the sebacic acid layers cause the aperiodic arrangement.


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