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**Supporting information for article:**

**Sulfur as hydrogen-bond acceptor in cocrystals of 2-thio-modified thymine**

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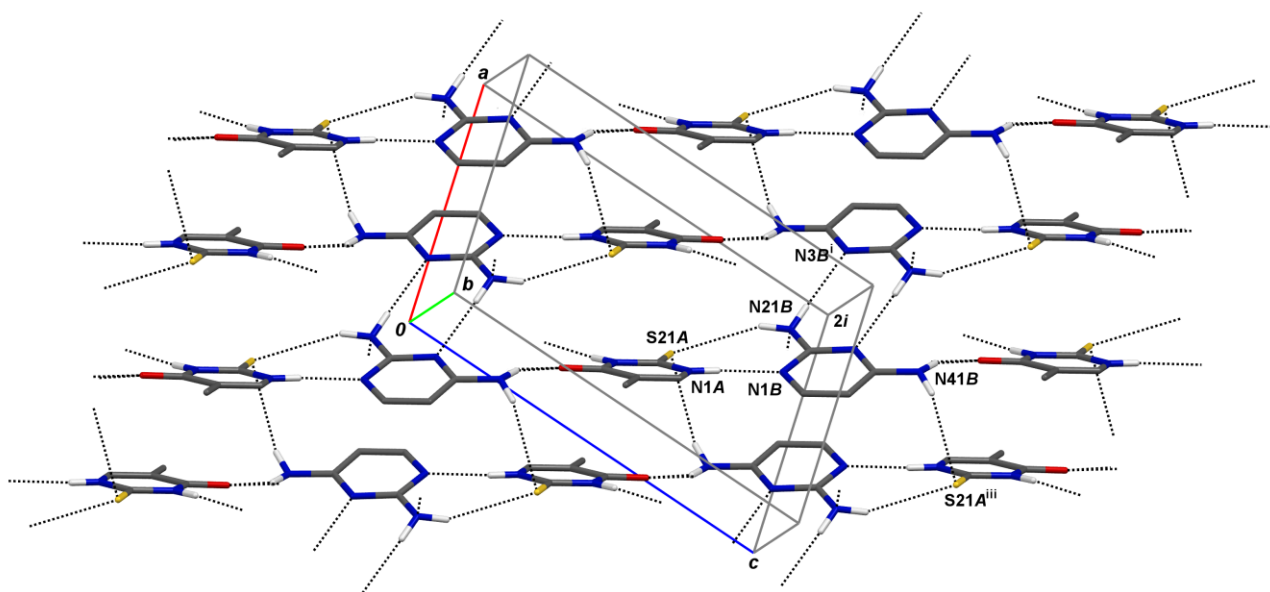


Fig. S1: A partial packing diagram for (I) showing the further connection of the chain-like arrangement shown in Fig. 3 yielding a three-dimensional network. Hydrogen bonds are shown as dashed lines. [Symmetry codes: (i)  $-x + 2, -y + 1, -z + 2$ ; (iii)  $-x + 1, -y + 1, -z + 2$ ].

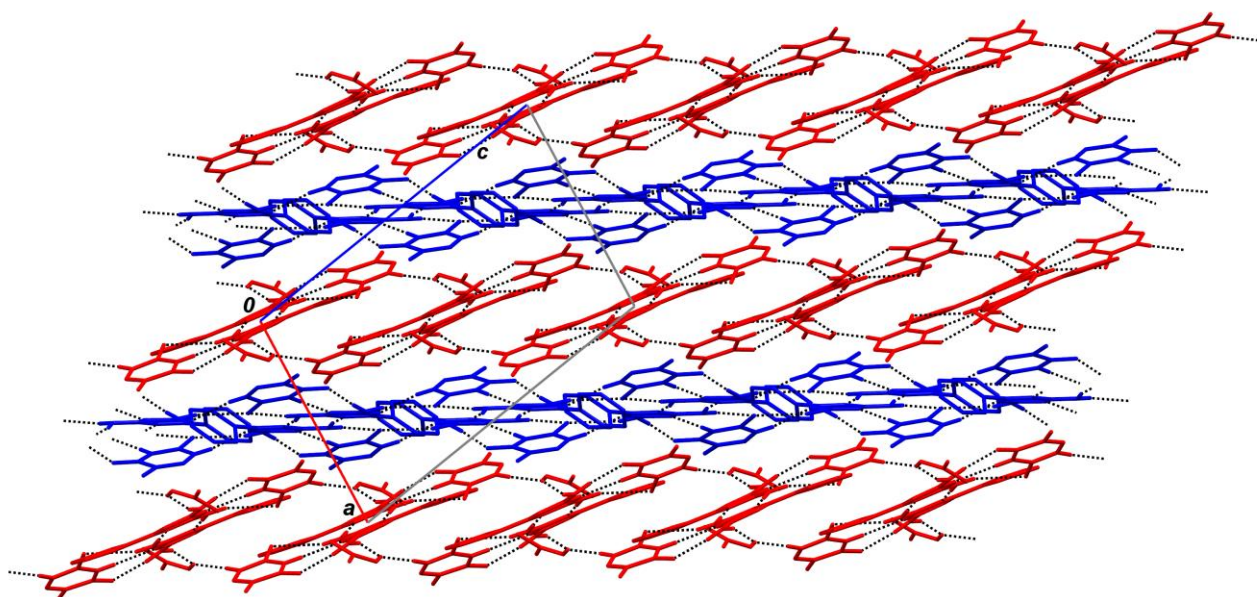


Figure S2: A packing diagram for (III) showing the alternating arrangement of DMF containing layers (red; molecules *B*, *D* and *X*) and solvent-free layers (blue; molecules *A* and *C*).

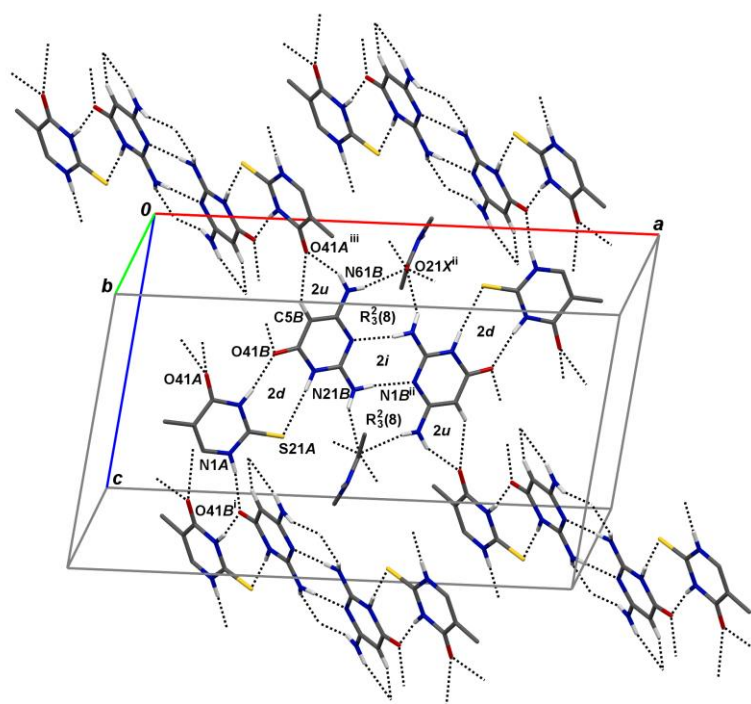


Figure S3: A partial packing diagram for (V). Hydrogen bonds are shown as dashed lines. Only one of the two equally occupied sites of the disordered DMAC molecule is shown [Symmetry codes: (i)  $x$ ,  $-y + 1$ ,  $z + 1/2$ ; (ii)  $-x + 1$ ,  $-y$ ,  $-z + 1$ ; (iii)  $-x + 1/2$ ,  $y - 1/2$ ,  $z + 1/2$ ].