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5-Fluorouracil–dimethyl sulfoxide (1/1)

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.090
Data-to-parameter ratio = 15.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_4H_3FN_2O_2\cdot C_2H_6OS$, crystallizes in the monoclinic space group $P2_1/c$, with one molecule of 5-fluorouracil and one molecule of dimethyl sulfoxide (DMSO) in the asymmetric unit. The crystal structure contains hydrogen-bonded ribbons of alternating 5-fluorouracil and DMSO molecules which stack, forming non-interacting layers parallel to the (100) planes.

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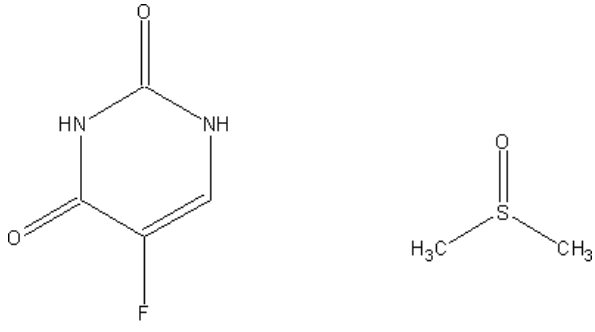
Comment

In the course of a polymorph screen performed on 5-fluorouracil three solvates were discovered; the crystal structure of one of these solvates is reported here. The title compound, (I), crystallizes in the space group $P2_1/c$ with one molecule of 5-fluorouracil and one molecule of dimethyl sulfoxide (DMSO) in the asymmetric unit.



(I)

The S atom in the DMSO molecule is disordered over two sites, with a 95:5 occupancy ratio. The minor site (S20′) exhibits the opposite pyrimidisation of the DMSO molecule, compared to the major site (S20). Fig. 1 shows the asymmetric unit, with only the major sulfur position shown.

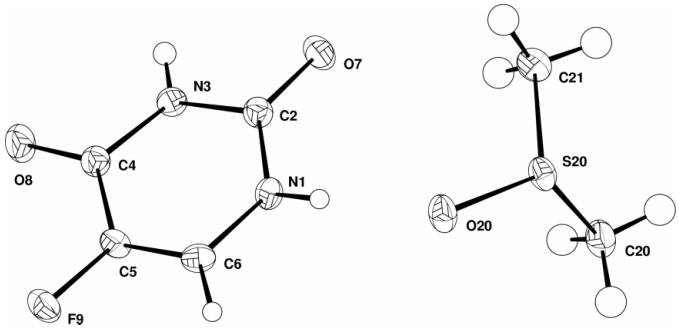


Figure 1
View (Watkin *et al.*, 1996) of the asymmetric unit of the title compound, with 50% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radii.

Two conventional hydrogen bonds, of the type N—H···O, occur in the structure. The O atom of the DMSO molecule acts as a hydrogen-bond acceptor for two symmetry-related 5-fluorouracil molecules (Table 1).

The crystal structure contains hydrogen-bonded ribbons of alternating 5-fluorouracil and DMSO molecules (Fig. 2). These ribbons stack, forming form non-interacting layers parallel to the (100) planes.

Experimental

5-Fluorouracil was obtained from the Aldrich Chemical Company Inc. The crystals of the title compound were grown by vapour diffusion of diethyl ether into a saturated solution of 5-fluorouracil in DMSO.

Crystal data

$C_4H_3FN_2O_2·C_2H_6OS$
$M_r = 208.21$
Monoclinic, $P2_1/c$
$a = 9.8831$ (10) Å
$b = 10.8128$ (11) Å
$c = 8.6842$ (9) Å
$\beta = 107.397$ (2)°
$V = 885.58$ (16) Å^3
$Z = 4$
$D_x = 1.562$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3031 reflections
$\theta = 2.9$–28.0°
$\mu = 0.36$ mm^{-1}
$T = 150$ (2) K
Block, colourless
0.29 × 0.21 × 0.11 mm

Data collection

Bruker SMART APEX diffractometer
Narrow-frame ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.903$, $T_{max} = 0.962$
7672 measured reflections
2128 independent reflections
1922 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 28.3°$
$h = -13 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.090$
$S = 1.07$
2127 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.5099P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.40$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O20	0.79 (2)	2.04 (2)	2.838 (2)	175 (2)
N3—H3···O20^{i}	0.82 (2)	1.97 (2)	2.790 (2)	173 (2)
N1—H1···S20$'$	0.79 (2)	2.56 (2)	3.266 (8)	149 (2)
N3—H3···S20^{i}	0.82 (2)	2.89 (2)	3.666 (1)	157 (2)

Symmetry code: (i) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$.

The S atom in the DMSO molecule is disordered over two sites and was modelled anisotropically, with site occupancy 95:5. The S—O and S—C distances in the major and minor components were restrained to be equal within ±0.01 Å. All H atoms on 5-fluorouracil were located in a difference map and were refined isotropically; N—H = 0.79 (2) and 0.82 (2) Å, and C—H = 0.94 (2) Å. The H-atom positions on the methyl group were idealized and refined using a riding model [C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$].

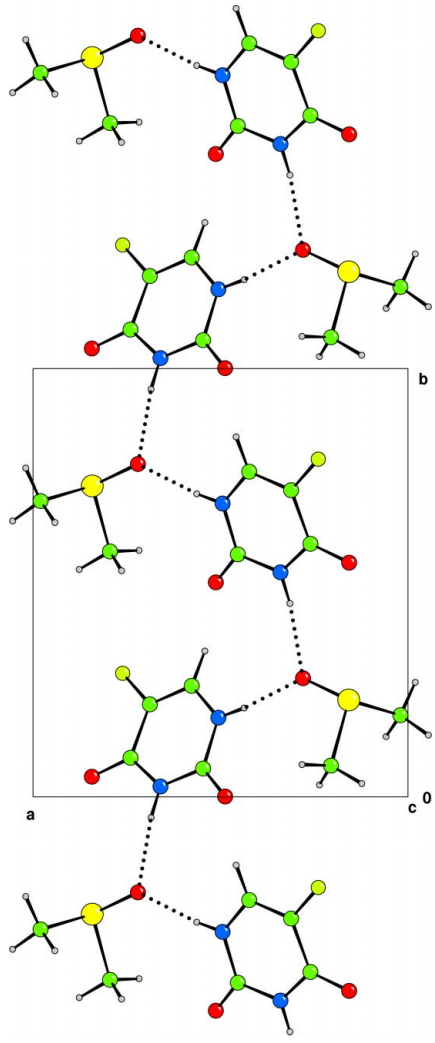


Figure 2
Hydrogen-bonded ribbon motif, made up of alternating 5-fluorouracil and DMSO molecules. Hydrogen bonds are shown as dashed lines.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *SHELXL*97.

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