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1-Pivaloyl-3-(pyrimidin-2-yl)thiourea

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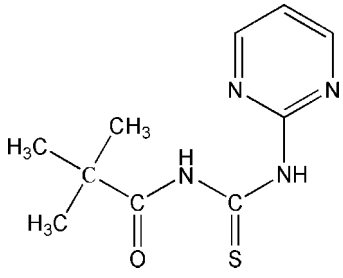
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.118; data-to-parameter ratio = 17.1.

There are two molecules in the asymmetric unit of the title compound, $C_{10}H_{14}N_4OS$. Both the thiocarbonyl and carbonyl groups are *cis* with respect to the C—N thiourea bond. Both intra- and intermolecular N—H···N hydrogen bonds stabilize the packing arrangement.

Related literature

For related literature, see: Allen (2002); Khawar Rauf, Badshah & Flörke (2006); Shoukat *et al.* (2007).



Experimental

Crystal data

$C_{10}H_{14}N_4OS$
M_r = 238.31
Triclinic, $P\overline{1}$
a = 5.652 (3) Å
b = 11.674 (8) Å
c = 18.585 (12) Å
α = 106.915 (9)°
β = 92.642 (6)°
γ = 94.478 (8)°
V = 1166.6 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 113 (2) K
0.45 × 0.36 × 0.20 mm

Data collection

Rigaku/MSC Mercury CCD diffractometer
Absorption correction: none
9547 measured reflections
5309 independent reflections
4314 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.118
S = 1.10
5309 reflections
311 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N4^{i}	0.86 (3)	2.27 (3)	3.133 (3)	174 (3)
N2—H2···N3	0.85 (3)	1.90 (3)	2.642 (3)	144 (3)
N5—H5···N8^{ii}	0.85 (3)	2.28 (3)	3.122 (3)	171 (2)
N6—H6···N7	0.86 (3)	1.88 (3)	2.632 (3)	144 (3)

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y, -z+1$.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *TEXSAN* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *TEXSAN*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2229).

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supplementary materials

Acta Cryst. (2007). E**63**, o2674 [**doi:10.1107/S1600536807019459**]

1-Pivaloyl-3-(pyrimidin-2-yl)thiourea

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Comment

The background to this study has been set out in our previous work for the structural chemistry of *N*,*N*′-disubstituted thioureas (Shoukat *et al.*, 2007). Herein, as a continuation of these studies, the structure of the title compound (I) is described. A depiction of the molecule is given in Fig. 1. Bond lengths and angles, see the selected geometric parameters table, can be regarded as typical for *N*,*N*′-disubstituted thiourea compounds as found in the Cambridge Structural Database v5.28 (Allen, 2002; Khawar Rauf *et al.*, 2006). The molecule exists in its thione form with typical thiourea C—S and C—O bond distances, as well as shortened C—N bonds (See geometric parameters table). The planes containing the S1, O1, N1, N2, C1 & C2 and S2, O2, N5, N6, C11 & C12 atoms are almost parallel to the pyrimidine ring, forming dihedral angles of 9.54 (13)° and 12.92 (12)° respectively. The molecules also feature intra & intermolecular N—H···N hydrogen bonds (See hydrogen-bond geometry table and Fig 2).

Experimental

Freshly prepared pivaloylisothiocyanate (1.43 g, 10 mmol) in acetone (30 ml) was stirred for 30 minutes. Neat 2-aminopyrimidine (1.0 g, 10 mmol) was then added and the resulting mixture was stirred for 1 h. The reaction mixture was poured into acidified water and stirred well. The solid product was separated and washed with deionized water and purified by recrystallization from methanol/ chloroform (1:5 *v/v*) to give fine crystals of (I), with an overall yield of 80%.

Refinement

C-bound H atoms were included in the riding model approximation with C—H 0.95–0.98 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) or U_{iso}(H) = 1.5 U_{eq}(C_{methyl}). The N-bound H atoms were refined isotropically.

Figures

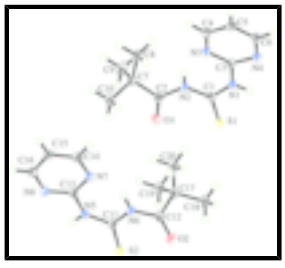

Fig. 1. Molecular structure of (I) showing the atom labelling scheme. Thermal displacement ellipsoids are drawn at the 50% probability level.

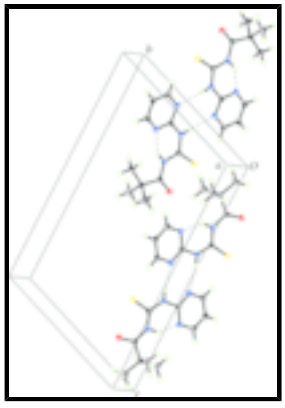

Fig. 2. Hydrogen-bonded dimer structures of (I) viewed along the *c*-axis. The hydrogen bonds are shown as dashed lines.

1-Pivaloyl-3-(pyrimidin-2-yl)thiourea

Crystal data

$C_{10}H_{14}N_4OS$	$Z = 4$
$M_r = 238.31$	$F_{000} = 504$
Triclinic, $P\bar{1}$	$D_x = 1.357$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 5.652$ (3) Å	Cell parameters from 3112 reflections
$b = 11.674$ (8) Å	$\theta = 3.3$–$27.5°$
$c = 18.585$ (12) Å	$\mu = 0.26$ mm^{-1}
$\alpha = 106.915$ (9)°	$T = 113$ (2) K
$\beta = 92.642$ (6)°	Block, yellow
$\gamma = 94.478$ (8)°	0.45 × 0.36 × 0.20 mm
$V = 1166.6$ (13) Å^3	

Data collection

Rigaku/MSC Mercury CCD diffractometer	5309 independent reflections
Radiation source: fine-focus sealed tube	4314 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.034$
Detector resolution: 14.62 pixels mm^{-1}	$\theta_{max} = 27.5°$
$T = 113(2)$ K	$\theta_{min} = 3.3°$
ω scans	$h = -7 \rightarrow 7$
Absorption correction: none	$k = -15 \rightarrow 9$
9547 measured reflections	$l = -18 \rightarrow 24$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 1.3663P]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.059$

$wR(F^2) = 0.118$

$S = 1.10$

5309 reflections

311 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}

$\Delta\rho_{min} = -0.32$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0618 (4)	0.4642 (2)	0.17088 (13)	0.0190 (5)
S1	−0.17984 (11)	0.37188 (6)	0.16735 (4)	0.02662 (16)
N1	0.1016 (3)	0.50531 (18)	0.10978 (11)	0.0197 (4)
H1	−0.010 (5)	0.480 (3)	0.0741 (17)	0.032 (8)*
C2	0.2483 (4)	0.4715 (2)	0.29593 (13)	0.0199 (5)
O1	0.1185 (3)	0.39231 (16)	0.30699 (10)	0.0307 (4)
N2	0.2299 (4)	0.50592 (18)	0.23032 (11)	0.0199 (4)
H2	0.339 (5)	0.555 (3)	0.2231 (16)	0.029 (8)*
C3	0.2906 (4)	0.5791 (2)	0.09625 (13)	0.0177 (5)
N3	0.4638 (3)	0.62528 (18)	0.15060 (11)	0.0214 (4)
C4	0.6480 (4)	0.6896 (2)	0.13348 (14)	0.0228 (5)
H4A	0.7752	0.7240	0.1706	0.027*
C5	0.6579 (4)	0.7071 (2)	0.06343 (14)	0.0231 (5)
H5A	0.7910	0.7504	0.0509	0.028*
C6	0.4640 (4)	0.6585 (2)	0.01227 (13)	0.0221 (5)
H6A	0.4640	0.6714	−0.0359	0.026*
N4	0.2768 (3)	0.59406 (18)	0.02747 (11)	0.0206 (4)
C7	0.4417 (4)	0.5426 (2)	0.35636 (13)	0.0217 (5)
C8	0.6106 (5)	0.6306 (2)	0.33193 (15)	0.0302 (6)
H8A	0.6919	0.5865	0.2884	0.045*
H8B	0.7285	0.6716	0.3736	0.045*
H8C	0.5197	0.6902	0.3181	0.045*

C9	0.3076 (5)	0.6119 (3)	0.42255 (15)	0.0338 (6)
H9A	0.4220	0.6566	0.4644	0.051*
H9B	0.2020	0.5552	0.4390	0.051*
H9C	0.2130	0.6683	0.4066	0.051*
C10	0.5839 (5)	0.4511 (3)	0.37960 (17)	0.0340 (6)
H10A	0.6701	0.4078	0.3370	0.051*
H10B	0.4748	0.3938	0.3944	0.051*
H10C	0.6976	0.4932	0.4223	0.051*
C11	0.2873 (4)	−0.0628 (2)	0.32001 (13)	0.0194 (5)
S2	0.05219 (11)	−0.15886 (6)	0.31716 (3)	0.02635 (16)
N5	0.4319 (3)	−0.01896 (18)	0.38563 (11)	0.0200 (4)
H5	0.386 (5)	−0.041 (2)	0.4230 (16)	0.021 (7)*
C12	0.2599 (4)	−0.0515 (2)	0.18742 (13)	0.0187 (5)
O2	0.1185 (3)	−0.13758 (16)	0.15963 (10)	0.0265 (4)
N6	0.3540 (4)	−0.01990 (19)	0.26246 (11)	0.0228 (5)
H6	0.470 (6)	0.037 (3)	0.2758 (18)	0.043 (9)*
C13	0.6386 (4)	0.0593 (2)	0.40249 (13)	0.0187 (5)
N7	0.7068 (4)	0.11528 (18)	0.35241 (11)	0.0219 (4)
C14	0.9128 (4)	0.1856 (2)	0.37013 (14)	0.0238 (5)
H14A	0.9672	0.2270	0.3360	0.029*
C15	1.0473 (4)	0.1998 (2)	0.43597 (14)	0.0243 (5)
H15A	1.1957	0.2478	0.4474	0.029*
C16	0.9569 (4)	0.1409 (2)	0.48524 (14)	0.0232 (5)
H16A	1.0452	0.1504	0.5317	0.028*
N8	0.7501 (3)	0.07114 (18)	0.46991 (11)	0.0210 (4)
C17	0.3594 (4)	0.0349 (2)	0.14560 (13)	0.0198 (5)
C18	0.2489 (5)	−0.0087 (3)	0.06439 (14)	0.0295 (6)
H18A	0.0753	−0.0106	0.0646	0.044*
H18B	0.2931	−0.0896	0.0398	0.044*
H18C	0.3076	0.0463	0.0368	0.044*
C19	0.6315 (4)	0.0367 (2)	0.14566 (14)	0.0233 (5)
H19A	0.6913	0.0878	0.1157	0.035*
H19B	0.6749	−0.0453	0.1238	0.035*
H19C	0.7021	0.0687	0.1976	0.035*
C20	0.2929 (4)	0.1612 (2)	0.18413 (15)	0.0262 (5)
H20A	0.3465	0.2154	0.1553	0.039*
H20B	0.3696	0.1900	0.2354	0.039*
H20C	0.1198	0.1593	0.1865	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0185 (11)	0.0198 (11)	0.0187 (12)	0.0015 (9)	−0.0006 (9)	0.0061 (9)
S1	0.0229 (3)	0.0307 (3)	0.0262 (3)	−0.0091 (3)	−0.0049 (2)	0.0124 (3)
N1	0.0176 (10)	0.0227 (10)	0.0183 (10)	−0.0048 (8)	−0.0051 (8)	0.0080 (8)
C2	0.0215 (11)	0.0200 (11)	0.0175 (11)	0.0007 (9)	0.0019 (9)	0.0048 (9)
O1	0.0358 (10)	0.0309 (10)	0.0266 (10)	−0.0112 (8)	−0.0034 (8)	0.0151 (8)
N2	0.0199 (10)	0.0208 (10)	0.0191 (10)	−0.0050 (8)	−0.0024 (8)	0.0084 (8)

C3	0.0166 (10)	0.0170 (11)	0.0185 (11)	−0.0009 (9)	−0.0024 (9)	0.0048 (9)
N3	0.0214 (10)	0.0226 (10)	0.0195 (10)	−0.0044 (8)	−0.0051 (8)	0.0079 (8)
C4	0.0200 (11)	0.0226 (12)	0.0247 (13)	−0.0030 (9)	−0.0041 (10)	0.0074 (10)
C5	0.0202 (12)	0.0233 (12)	0.0250 (13)	−0.0056 (10)	−0.0023 (10)	0.0082 (10)
C6	0.0254 (12)	0.0240 (12)	0.0168 (12)	−0.0017 (10)	−0.0010 (9)	0.0076 (10)
N4	0.0204 (10)	0.0211 (10)	0.0196 (10)	−0.0024 (8)	−0.0018 (8)	0.0064 (8)
C7	0.0204 (11)	0.0259 (12)	0.0192 (12)	−0.0004 (10)	−0.0016 (9)	0.0081 (10)
C8	0.0297 (13)	0.0345 (15)	0.0257 (14)	−0.0107 (11)	−0.0079 (11)	0.0128 (12)
C9	0.0361 (15)	0.0399 (16)	0.0205 (13)	0.0007 (12)	−0.0014 (11)	0.0023 (12)
C10	0.0252 (13)	0.0451 (17)	0.0395 (17)	0.0043 (12)	−0.0023 (12)	0.0249 (14)
C11	0.0205 (11)	0.0211 (11)	0.0162 (11)	−0.0020 (9)	−0.0018 (9)	0.0063 (9)
S2	0.0259 (3)	0.0327 (3)	0.0196 (3)	−0.0122 (3)	−0.0041 (2)	0.0112 (3)
N5	0.0212 (10)	0.0236 (10)	0.0163 (10)	−0.0053 (8)	−0.0017 (8)	0.0098 (8)
C12	0.0164 (11)	0.0247 (12)	0.0148 (11)	0.0019 (9)	0.0015 (9)	0.0057 (9)
O2	0.0268 (9)	0.0295 (10)	0.0202 (9)	−0.0101 (8)	−0.0032 (7)	0.0065 (7)
N6	0.0239 (11)	0.0258 (11)	0.0184 (10)	−0.0089 (9)	−0.0041 (8)	0.0101 (9)
C13	0.0204 (11)	0.0189 (11)	0.0159 (11)	−0.0014 (9)	−0.0002 (9)	0.0048 (9)
N7	0.0240 (10)	0.0233 (10)	0.0182 (10)	−0.0054 (8)	−0.0015 (8)	0.0084 (8)
C14	0.0269 (12)	0.0230 (12)	0.0215 (12)	−0.0029 (10)	0.0026 (10)	0.0077 (10)
C15	0.0231 (12)	0.0237 (12)	0.0238 (13)	−0.0065 (10)	0.0004 (10)	0.0062 (10)
C16	0.0236 (12)	0.0230 (12)	0.0205 (12)	−0.0018 (10)	−0.0021 (9)	0.0040 (10)
N8	0.0209 (10)	0.0236 (10)	0.0178 (10)	−0.0011 (8)	−0.0013 (8)	0.0064 (8)
C17	0.0156 (11)	0.0269 (12)	0.0186 (12)	−0.0002 (9)	−0.0008 (9)	0.0105 (10)
C18	0.0251 (13)	0.0475 (16)	0.0176 (12)	−0.0026 (12)	−0.0007 (10)	0.0143 (12)
C19	0.0187 (11)	0.0300 (13)	0.0226 (13)	0.0019 (10)	0.0014 (9)	0.0102 (10)
C20	0.0248 (12)	0.0291 (13)	0.0291 (14)	0.0033 (10)	0.0041 (10)	0.0148 (11)

Geometric parameters (Å, °)

C1—N2	1.371 (3)	C11—N6	1.362 (3)
C1—N1	1.376 (3)	C11—N5	1.377 (3)
C1—S1	1.659 (2)	C11—S2	1.659 (2)
N1—C3	1.397 (3)	N5—C13	1.390 (3)
N1—H1	0.86 (3)	N5—H5	0.85 (3)
C2—O1	1.206 (3)	C12—O2	1.204 (3)
C2—N2	1.392 (3)	C12—N6	1.402 (3)
C2—C7	1.532 (3)	C12—C17	1.531 (3)
N2—H2	0.85 (3)	N6—H6	0.86 (3)
C3—N3	1.334 (3)	C13—N7	1.338 (3)
C3—N4	1.339 (3)	C13—N8	1.341 (3)
N3—C4	1.340 (3)	N7—C14	1.340 (3)
C4—C5	1.378 (3)	C14—C15	1.371 (4)
C4—H4A	0.9500	C14—H14A	0.9500
C5—C6	1.385 (3)	C15—C16	1.388 (3)
C5—H5A	0.9500	C15—H15A	0.9500
C6—N4	1.338 (3)	C16—N8	1.340 (3)
C6—H6A	0.9500	C16—H16A	0.9500
C7—C8	1.527 (3)	C17—C20	1.525 (4)
C7—C10	1.531 (4)	C17—C18	1.531 (3)

C7—C9	1.531 (4)	C17—C19	1.537 (3)
C8—H8A	0.9800	C18—H18A	0.9800
C8—H8B	0.9800	C18—H18B	0.9800
C8—H8C	0.9800	C18—H18C	0.9800
C9—H9A	0.9800	C19—H19A	0.9800
C9—H9B	0.9800	C19—H19B	0.9800
C9—H9C	0.9800	C19—H19C	0.9800
C10—H10A	0.9800	C20—H20A	0.9800
C10—H10B	0.9800	C20—H20B	0.9800
C10—H10C	0.9800	C20—H20C	0.9800
N2—C1—N1	115.3 (2)	N6—C11—N5	114.8 (2)
N2—C1—S1	125.97 (18)	N6—C11—S2	125.95 (18)
N1—C1—S1	118.74 (17)	N5—C11—S2	119.27 (17)
C1—N1—C3	131.0 (2)	C11—N5—C13	130.8 (2)
C1—N1—H1	113.4 (19)	C11—N5—H5	115.6 (18)
C3—N1—H1	115.6 (19)	C13—N5—H5	113.6 (18)
O1—C2—N2	123.3 (2)	O2—C12—N6	123.2 (2)
O1—C2—C7	120.3 (2)	O2—C12—C17	124.5 (2)
N2—C2—C7	116.36 (19)	N6—C12—C17	112.29 (19)
C1—N2—C2	127.9 (2)	C11—N6—C12	129.9 (2)
C1—N2—H2	113.3 (19)	C11—N6—H6	113 (2)
C2—N2—H2	118.6 (19)	C12—N6—H6	117 (2)
N3—C3—N4	126.9 (2)	N7—C13—N8	126.4 (2)
N3—C3—N1	118.6 (2)	N7—C13—N5	119.0 (2)
N4—C3—N1	114.45 (19)	N8—C13—N5	114.59 (19)
C3—N3—C4	116.5 (2)	C13—N7—C14	116.5 (2)
N3—C4—C5	121.8 (2)	N7—C14—C15	122.1 (2)
N3—C4—H4A	119.1	N7—C14—H14A	119.0
C5—C4—H4A	119.1	C15—C14—H14A	119.0
C4—C5—C6	116.7 (2)	C14—C15—C16	117.0 (2)
C4—C5—H5A	121.6	C14—C15—H15A	121.5
C6—C5—H5A	121.6	C16—C15—H15A	121.5
N4—C6—C5	123.1 (2)	N8—C16—C15	122.7 (2)
N4—C6—H6A	118.4	N8—C16—H16A	118.7
C5—C6—H6A	118.4	C15—C16—H16A	118.7
C6—N4—C3	114.94 (19)	C16—N8—C13	115.3 (2)
C8—C7—C10	109.6 (2)	C20—C17—C18	109.8 (2)
C8—C7—C9	109.5 (2)	C20—C17—C12	109.4 (2)
C10—C7—C9	110.1 (2)	C18—C17—C12	108.02 (19)
C8—C7—C2	114.9 (2)	C20—C17—C19	109.41 (19)
C10—C7—C2	107.3 (2)	C18—C17—C19	109.7 (2)
C9—C7—C2	105.3 (2)	C12—C17—C19	110.48 (19)
C7—C8—H8A	109.5	C17—C18—H18A	109.5
C7—C8—H8B	109.5	C17—C18—H18B	109.5
H8A—C8—H8B	109.5	H18A—C18—H18B	109.5
C7—C8—H8C	109.5	C17—C18—H18C	109.5
H8A—C8—H8C	109.5	H18A—C18—H18C	109.5
H8B—C8—H8C	109.5	H18B—C18—H18C	109.5
C7—C9—H9A	109.5	C17—C19—H19A	109.5

C7—C9—H9B	109.5	C17—C19—H19B	109.5
H9A—C9—H9B	109.5	H19A—C19—H19B	109.5
C7—C9—H9C	109.5	C17—C19—H19C	109.5
H9A—C9—H9C	109.5	H19A—C19—H19C	109.5
H9B—C9—H9C	109.5	H19B—C19—H19C	109.5
C7—C10—H10A	109.5	C17—C20—H20A	109.5
C7—C10—H10B	109.5	C17—C20—H20B	109.5
H10A—C10—H10B	109.5	H20A—C20—H20B	109.5
C7—C10—H10C	109.5	C17—C20—H20C	109.5
H10A—C10—H10C	109.5	H20A—C20—H20C	109.5
H10B—C10—H10C	109.5	H20B—C20—H20C	109.5
N2—C1—N1—C3	3.1 (4)	N6—C11—N5—C13	−2.0 (4)
S1—C1—N1—C3	−177.5 (2)	S2—C11—N5—C13	178.7 (2)
N1—C1—N2—C2	−173.5 (2)	N5—C11—N6—C12	174.7 (2)
S1—C1—N2—C2	7.1 (4)	S2—C11—N6—C12	−6.0 (4)
O1—C2—N2—C1	4.1 (4)	O2—C12—N6—C11	−10.9 (4)
C7—C2—N2—C1	−174.2 (2)	C17—C12—N6—C11	169.7 (2)
C1—N1—C3—N3	−3.5 (4)	C11—N5—C13—N7	8.3 (4)
C1—N1—C3—N4	175.7 (2)	C11—N5—C13—N8	−172.2 (2)
N4—C3—N3—C4	−2.9 (4)	N8—C13—N7—C14	3.4 (4)
N1—C3—N3—C4	176.2 (2)	N5—C13—N7—C14	−177.2 (2)
C3—N3—C4—C5	0.1 (4)	C13—N7—C14—C15	0.0 (4)
N3—C4—C5—C6	2.1 (4)	N7—C14—C15—C16	−2.1 (4)
C4—C5—C6—N4	−2.0 (4)	C14—C15—C16—N8	1.1 (4)
C5—C6—N4—C3	−0.4 (4)	C15—C16—N8—C13	1.8 (4)
N3—C3—N4—C6	3.0 (4)	N7—C13—N8—C16	−4.2 (4)
N1—C3—N4—C6	−176.1 (2)	N5—C13—N8—C16	176.3 (2)
O1—C2—C7—C8	173.6 (2)	O2—C12—C17—C20	119.2 (3)
N2—C2—C7—C8	−8.0 (3)	N6—C12—C17—C20	−61.4 (3)
O1—C2—C7—C10	51.5 (3)	O2—C12—C17—C18	−0.3 (3)
N2—C2—C7—C10	−130.1 (2)	N6—C12—C17—C18	179.1 (2)
O1—C2—C7—C9	−65.8 (3)	O2—C12—C17—C19	−120.3 (3)
N2—C2—C7—C9	112.6 (2)	N6—C12—C17—C19	59.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···N4^{i}	0.86 (3)	2.27 (3)	3.133 (3)	174 (3)
N2—H2···N3	0.85 (3)	1.90 (3)	2.642 (3)	144 (3)
N5—H5···N8^{ii}	0.85 (3)	2.28 (3)	3.122 (3)	171 (2)
N6—H6···N7	0.86 (3)	1.88 (3)	2.632 (3)	144 (3)

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*+1.

Fig. 1

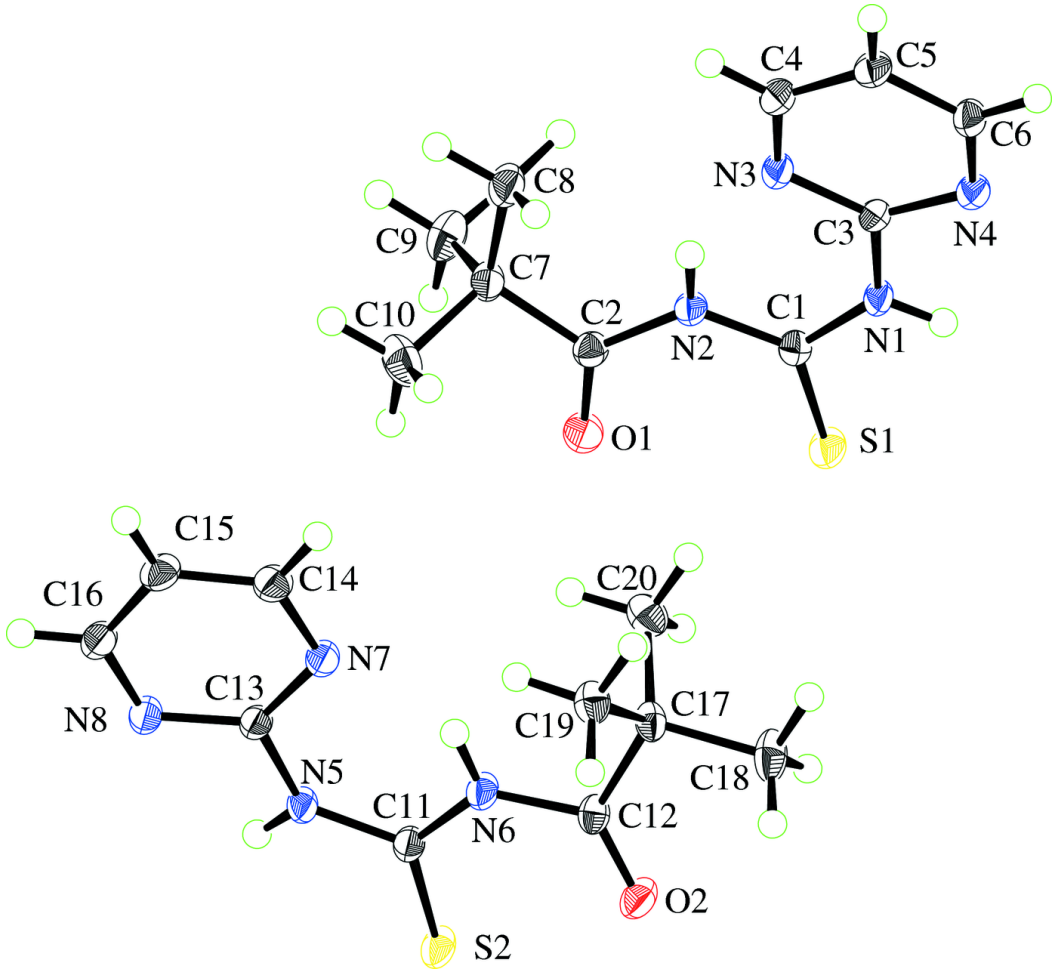
C4
C5
C6
N3
N4
C3
C8
C9
C7
C10
C2
N2
C1
N1
O1
S1
C15
C14
C16
N7
C13
N8
C20
C19
C17
C18
N5
C11
N6
C12
O2
S2

Fig. 2