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2-[3-(2-Methylbenzoyl)thioureido]-3-phenylpropionic acid

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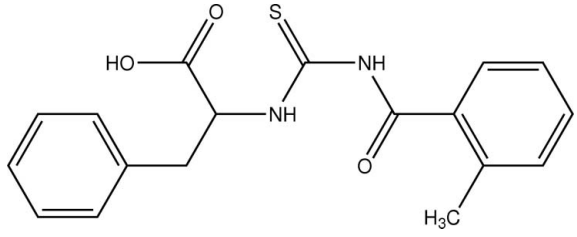
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.096; data-to-parameter ratio = 15.4.

In the title compound, $C_{18}H_{18}N_2O_3S$, the central thiourea and 2-methylphenyl fragments make a dihedral angle of 55.40 (7)°. In the crystal structure, molecules are stabilized by intermolecular O—H···S, N—H···O and C—H···O hydrogen bonds, forming a one-dimensional chain along the *a* axis.

Related literature

For structures analogous to the title compound, see: Ngah *et al.* (2005). For details of the normal bond lengths and angles found in the title compound, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{18}N_2O_3S$
M_r = 342.40
Orthorhombic, $P2_12_12_1$
a = 7.4377 (16) Å
b = 24.554 (5) Å
c = 9.385 (2) Å
V = 1713.9 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 (2) K
0.50 × 0.38 × 0.29 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.904, T_{max} = 0.942
9565 measured reflections
3339 independent reflections
3111 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.096
S = 0.98
3339 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 1396 Freidel pairs
Flack parameter: 0.08 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	1.95	2.636 (2)	135
C9—H9A···S1	0.98	2.60	3.091 (2)	111
C20—H20B···O1	0.96	2.54	2.994 (3)	109
C1—H1B···O2^{i}	0.93	2.50	3.187 (3)	130
C2—H2B···O1^{i}	0.93	2.50	3.409 (3)	165
N1—H1A···O2^{i}	0.86	2.46	3.237 (2)	150
O3—H3···S1^{ii}	0.80	2.34	3.1361 (17)	177
C9—H9A···O2^{iii}	0.98	2.58	3.338 (2)	134

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $-x+\frac{1}{2}, -y+2, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2353).

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supplementary materials

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2-[3-(2-Methylbenzoyl)thioureido]-3-phenylpropionic acid

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Comment

The title compound, (I), is an amino acids derivative of thiourea and analoguos with 2-[3-(4-methoxybenzoyl)thioureido-3-phenylpropionic acid methanol solvate, (II), (Ngah *et al.*, 2005), except that the position of methyl group at the phenyl ring (Fig.1). The molecule maintains its *trans-cis* configuration with respect to the positions of 2-methylbenzoyl and 3-phenylpropionic acid relative to the S1 atom across the C8—N1 and C8—N2 bonds, respectively. The bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and are comparable to those in (II). The central thiourea (S1/N1/N2/C8), 2-methylphenyl (C1–C6/C20) and phenyl ring (C11–C16) fragments are essentially planar with a maximum deviation of 0.041 (2) Å for atom C7 from the least square planes. The dihedral angles between the central thiourea and 2-methylphenyl fragments is 55.40 (7)°.

There are three intramolecular N—H···O, C—H···S and C—H···O hydrogen bonds, (Table 2), and as a result, a pseudo-five- (S1···H9—C9—N2—C8—S1) and two pseudo-six membered rings (O1···H2—N2—C8—N1—C7—O1), (O1···H20—C20—C5—C6—C7—O1) are formed. In the crystal structure the molecules are stabilized by intermolecular O—H···S, N—H···O and C—H···O hydrogen bonds, (Table 2), forming a one-dimensional chain along to *a* axis (Fig.2).

Experimental

A solution of *L*-phenylalanine in acetone was added dropwise to a two-necked round-bottomed flask containing an equimolar solution of 2-methylbenzoyl isothiocyanate in distilled acetone. The mixture was refluxed for about 5 h to complete the reaction. The resulting solution was poured into a beaker containing some ice cubes. The white precipitate obtained was filtered and washed with distilled water and cold ethanol before dried under vacuum. Good quality crystals of (I) were obtained by recrystallization from methanol (yield 81%, m.p. 385.2–386.4 K).

Refinement

After their location in the difference map, all H-atoms were fixed geometrically at ideal positions and allowed to ride on the parent C, N or O atoms with C—H = 0.93–0.97 Å, N—H = 0.86Å and O—H = 0.80 Å, with U_{iso}(H)= 1.2Ueq(C, N) and 1.5Ueq (C_{methyl}, $O_{hydroxyl}$).

Figures

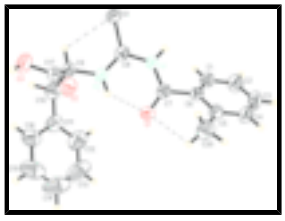

Fig. 1. Molecular structure of the title compound (I), with the 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bonds.

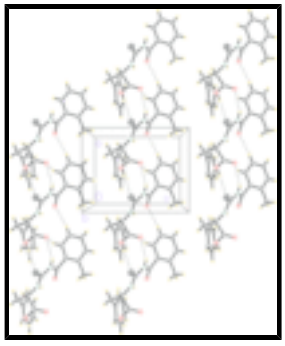

Fig. 2. Packing diagram of compound (I), viewed down the *b* axis. The dashed lines denote the intermolecular N—H···O, O—H···S and C—H···O hydrogen bonds.

2-[3-(2-Methylbenzoyl)thioureido]-3-phenylpropionic acid

Crystal data

$C_{18}H_{18}N_2O_3S$	F_{000} = 720
M_r = 342.40	D_x = 1.327 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 947 reflections
a = 7.4377 (16) Å	θ = 1.6–25.9º
b = 24.554 (5) Å	μ = 0.21 mm^{-1}
c = 9.385 (2) Å	T = 293 (2) K
V = 1713.9 (6) Å^3	Block, colourless
Z = 4	0.50 × 0.38 × 0.29 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	3339 independent reflections
Radiation source: fine-focus sealed tube	3111 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.018
Detector resolution: 83.66 pixels mm^{-1}	θ_{max} = 25.9º
T = 293(2) K	θ_{min} = 1.6º
ω scans	h = −8→9
Absorption correction: multi-scan (SADABS; Bruker, 2000)	k = −30→23
T_{min} = 0.904, T_{max} = 0.942	l = −11→11
9565 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.1974P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.096	$(\Delta/\sigma)_{max} < 0.001$

S = 0.98	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
3339 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
217 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1396 Freidel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.08 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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}
S1	−0.13853 (7)	1.026957 (19)	1.05397 (6)	0.05106 (16)
N1	−0.18460 (19)	0.93256 (6)	0.92189 (17)	0.0384 (3)
H1A	−0.2862	0.9468	0.8991	0.046*
O1	−0.00976 (19)	0.85763 (6)	0.89046 (16)	0.0540 (4)
C8	−0.0772 (2)	0.96311 (7)	1.01294 (19)	0.0381 (4)
O2	0.4010 (2)	0.96999 (6)	0.96043 (15)	0.0516 (3)
N2	0.0706 (2)	0.93940 (6)	1.06088 (19)	0.0452 (4)
H2A	0.0935	0.9069	1.0317	0.054*
C17	0.3630 (3)	0.98307 (7)	1.0794 (2)	0.0423 (4)
C7	−0.1486 (3)	0.88225 (7)	0.86356 (19)	0.0387 (4)
C5	−0.2457 (3)	0.83614 (8)	0.6372 (2)	0.0422 (4)
O3	0.4643 (2)	1.01424 (7)	1.16113 (17)	0.0622 (4)
C1	−0.4677 (3)	0.85934 (8)	0.8167 (2)	0.0456 (4)
H1B	−0.4959	0.8754	0.9036	0.055*
C6	−0.2909 (3)	0.85943 (7)	0.76887 (19)	0.0373 (4)
C9	0.1965 (3)	0.96422 (8)	1.1589 (2)	0.0448 (5)
H9A	0.1388	0.9961	1.2021	0.054*
C11	0.3542 (4)	0.87540 (8)	1.2309 (2)	0.0520 (5)
C4	−0.3840 (3)	0.81296 (9)	0.5593 (2)	0.0531 (5)
H4A	−0.3579	0.7974	0.4714	0.064*
C10	0.2496 (3)	0.92471 (9)	1.2782 (2)	0.0526 (5)
H10A	0.3209	0.9444	1.3477	0.063*
H10B	0.1410	0.9125	1.3256	0.063*
C2	−0.6009 (3)	0.83567 (10)	0.7367 (3)	0.0588 (6)
H2B	−0.7188	0.8355	0.7695	0.071*
C3	−0.5594 (3)	0.81220 (10)	0.6076 (3)	0.0625 (6)

H3A	−0.6490	0.7959	0.5532	0.075*
C20	−0.0583 (3)	0.83576 (10)	0.5790 (2)	0.0613 (6)
H20A	−0.0576	0.8179	0.4879	0.092*
H20B	0.0194	0.8166	0.6434	0.092*
H20C	−0.0166	0.8725	0.5682	0.092*
C16	0.5398 (4)	0.87715 (10)	1.2231 (2)	0.0615 (6)
H16A	0.6000	0.9090	1.2477	0.074*
C12	0.2681 (5)	0.82709 (10)	1.1949 (3)	0.0745 (8)
H12A	0.1435	0.8249	1.2002	0.089*
C13	0.3668 (7)	0.78194 (11)	1.1511 (3)	0.1000 (12)
H13A	0.3081	0.7499	1.1262	0.120*
C14	0.5507 (7)	0.78483 (14)	1.1446 (3)	0.1008 (13)
H14A	0.6165	0.7545	1.1166	0.121*
C15	0.6375 (5)	0.83178 (13)	1.1789 (3)	0.0850 (9)
H15B	0.7622	0.8336	1.1728	0.102*
H3	0.5643	1.0178	1.1310	0.128*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0447 (3)	0.0341 (2)	0.0744 (3)	−0.0009 (2)	−0.0013 (2)	−0.0124 (2)
N1	0.0348 (8)	0.0341 (7)	0.0461 (8)	−0.0001 (6)	−0.0029 (6)	−0.0047 (6)
O1	0.0457 (8)	0.0498 (8)	0.0665 (9)	0.0125 (7)	−0.0129 (7)	−0.0214 (7)
C8	0.0340 (9)	0.0383 (9)	0.0420 (9)	−0.0040 (7)	0.0056 (7)	−0.0040 (7)
O2	0.0557 (9)	0.0550 (8)	0.0440 (7)	−0.0029 (7)	−0.0019 (6)	−0.0021 (6)
N2	0.0394 (8)	0.0415 (8)	0.0546 (9)	0.0034 (6)	−0.0058 (8)	−0.0165 (7)
C17	0.0452 (10)	0.0340 (9)	0.0478 (10)	0.0043 (8)	−0.0074 (9)	−0.0035 (8)
C7	0.0391 (10)	0.0390 (9)	0.0380 (8)	0.0006 (8)	0.0030 (8)	−0.0044 (7)
C5	0.0486 (11)	0.0396 (9)	0.0382 (9)	0.0017 (8)	−0.0021 (8)	0.0010 (8)
O3	0.0520 (9)	0.0669 (10)	0.0677 (9)	−0.0151 (7)	−0.0005 (8)	−0.0245 (8)
C1	0.0429 (11)	0.0488 (11)	0.0452 (10)	−0.0003 (8)	0.0022 (8)	−0.0066 (8)
C6	0.0429 (10)	0.0309 (8)	0.0381 (9)	0.0005 (7)	−0.0031 (7)	−0.0012 (7)
C9	0.0405 (10)	0.0455 (11)	0.0485 (10)	0.0016 (8)	−0.0031 (8)	−0.0161 (8)
C11	0.0739 (15)	0.0472 (10)	0.0349 (9)	−0.0004 (10)	−0.0011 (10)	0.0051 (8)
C4	0.0633 (14)	0.0558 (11)	0.0401 (10)	−0.0019 (10)	−0.0063 (10)	−0.0105 (9)
C10	0.0519 (12)	0.0644 (13)	0.0414 (10)	−0.0060 (10)	0.0045 (9)	−0.0080 (9)
C2	0.0372 (12)	0.0717 (14)	0.0677 (13)	−0.0046 (10)	−0.0002 (10)	−0.0099 (12)
C3	0.0528 (13)	0.0717 (15)	0.0631 (14)	−0.0060 (11)	−0.0179 (11)	−0.0163 (11)
C20	0.0571 (13)	0.0737 (14)	0.0530 (12)	−0.0055 (11)	0.0107 (11)	−0.0135 (11)
C16	0.0757 (17)	0.0606 (14)	0.0482 (11)	0.0121 (12)	−0.0019 (11)	0.0065 (10)
C12	0.109 (2)	0.0534 (15)	0.0612 (15)	−0.0117 (14)	−0.0116 (15)	0.0098 (12)
C13	0.186 (4)	0.0415 (14)	0.0725 (18)	−0.001 (2)	−0.017 (3)	0.0040 (12)
C14	0.179 (4)	0.0629 (19)	0.0608 (16)	0.046 (2)	0.006 (2)	0.0088 (14)
C15	0.106 (2)	0.089 (2)	0.0592 (15)	0.041 (2)	0.0097 (16)	0.0165 (15)

Geometric parameters (Å, °)

S1—C8	1.6775 (18)	C11—C12	1.389 (3)
N1—C7	1.377 (2)	C11—C10	1.506 (3)

N1—C8	1.390 (2)	C4—C3	1.381 (3)
N1—H1A	0.8600	C4—H4A	0.9300
O1—C7	1.223 (2)	C10—H10A	0.9700
C8—N2	1.323 (3)	C10—H10B	0.9700
O2—C17	1.196 (2)	C2—C3	1.377 (3)
N2—C9	1.447 (2)	C2—H2B	0.9300
N2—H2A	0.8600	C3—H3A	0.9300
C17—O3	1.320 (2)	C20—H20A	0.9600
O3—H3	0.8000	C20—H20B	0.9600
C17—C9	1.518 (3)	C20—H20C	0.9600
C7—C6	1.491 (3)	C16—C15	1.393 (4)
C5—C4	1.385 (3)	C16—H16A	0.9300
C5—C6	1.402 (3)	C12—C13	1.392 (5)
C5—C20	1.497 (3)	C12—H12A	0.9300
C1—C2	1.372 (3)	C13—C14	1.370 (5)
C1—C6	1.389 (3)	C13—H13A	0.9300
C1—H1B	0.9300	C14—C15	1.360 (5)
C9—C10	1.533 (3)	C14—H14A	0.9300
C9—H9A	0.9800	C15—H15B	0.9300
C11—C16	1.383 (4)		
C17—O3—H3	113.00	C5—C4—H4A	118.9
C7—N1—C8	128.09 (16)	C11—C10—C9	115.26 (16)
C7—N1—H1A	116.0	C11—C10—H10A	108.5
C8—N1—H1A	116.0	C9—C10—H10A	108.5
N2—C8—N1	116.69 (16)	C11—C10—H10B	108.5
N2—C8—S1	124.00 (14)	C9—C10—H10B	108.5
N1—C8—S1	119.31 (14)	H10A—C10—H10B	107.5
C8—N2—C9	124.64 (15)	C1—C2—C3	119.8 (2)
C8—N2—H2A	117.7	C1—C2—H2B	120.1
C9—N2—H2A	117.7	C3—C2—H2B	120.1
O2—C17—O3	124.3 (2)	C2—C3—C4	119.7 (2)
O2—C17—C9	124.73 (17)	C2—C3—H3A	120.2
O3—C17—C9	110.95 (16)	C4—C3—H3A	120.2
O1—C7—N1	121.69 (17)	C5—C20—H20A	109.5
O1—C7—C6	122.44 (16)	C5—C20—H20B	109.5
N1—C7—C6	115.85 (16)	H20A—C20—H20B	109.5
C4—C5—C6	117.07 (19)	C5—C20—H20C	109.5
C4—C5—C20	119.74 (18)	H20A—C20—H20C	109.5
C6—C5—C20	123.18 (18)	H20B—C20—H20C	109.5
C2—C1—C6	120.47 (19)	C11—C16—C15	120.8 (3)
C2—C1—H1B	119.8	C11—C16—H16A	119.6
C6—C1—H1B	119.8	C15—C16—H16A	119.6
C1—C6—C5	120.71 (18)	C11—C12—C13	120.6 (3)
C1—C6—C7	118.66 (16)	C11—C12—H12A	119.7
C5—C6—C7	120.56 (17)	C13—C12—H12A	119.7
N2—C9—C17	110.12 (16)	C14—C13—C12	119.9 (3)
N2—C9—C10	111.37 (17)	C14—C13—H13A	120.1
C17—C9—C10	109.96 (16)	C12—C13—H13A	120.1
N2—C9—H9A	108.4	C15—C14—C13	120.5 (3)

C17—C9—H9A	108.4	C15—C14—H14A	119.8
C10—C9—H9A	108.4	C13—C14—H14A	119.8
C16—C11—C12	118.3 (2)	C14—C15—C16	120.0 (4)
C16—C11—C10	120.4 (2)	C14—C15—H15B	120.0
C12—C11—C10	121.3 (3)	C16—C15—H15B	120.0
C3—C4—C5	122.27 (19)	C14—C15—H3	139.4
C3—C4—H4A	118.9	H15B—C15—H3	93.7
C7—N1—C8—N2	−6.9 (3)	O2—C17—C9—C10	109.4 (2)
C7—N1—C8—S1	172.36 (15)	O3—C17—C9—C10	−68.2 (2)
N1—C8—N2—C9	−178.50 (18)	C6—C5—C4—C3	−0.3 (3)
S1—C8—N2—C9	2.3 (3)	C20—C5—C4—C3	−179.9 (2)
C8—N1—C7—O1	1.3 (3)	C16—C11—C10—C9	88.8 (2)
C8—N1—C7—C6	179.99 (17)	C12—C11—C10—C9	−91.7 (2)
C2—C1—C6—C5	1.0 (3)	N2—C9—C10—C11	65.7 (2)
C2—C1—C6—C7	−175.9 (2)	C17—C9—C10—C11	−56.7 (2)
C4—C5—C6—C1	−0.6 (3)	C6—C1—C2—C3	−0.5 (3)
C20—C5—C6—C1	179.0 (2)	C1—C2—C3—C4	−0.4 (4)
C4—C5—C6—C7	176.29 (17)	C5—C4—C3—C2	0.8 (4)
C20—C5—C6—C7	−4.1 (3)	C12—C11—C16—C15	0.7 (3)
O1—C7—C6—C1	129.8 (2)	C10—C11—C16—C15	−179.7 (2)
N1—C7—C6—C1	−48.8 (2)	C16—C11—C12—C13	−0.6 (4)
O1—C7—C6—C5	−47.1 (3)	C10—C11—C12—C13	179.8 (2)
N1—C7—C6—C5	134.26 (18)	C11—C12—C13—C14	0.7 (4)
C8—N2—C9—C17	−103.6 (2)	C12—C13—C14—C15	−0.9 (5)
C8—N2—C9—C10	134.17 (19)	C13—C14—C15—C16	1.0 (5)
O2—C17—C9—N2	−13.7 (3)	C11—C16—C15—C14	−0.9 (4)
O3—C17—C9—N2	168.75 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O1	0.86	1.95	2.636 (2)	135
C9—H9A···S1	0.98	2.60	3.091 (2)	111
C20—H20B···O1	0.96	2.54	2.994 (3)	109
C1—H1B···O2^{i}	0.93	2.50	3.187 (3)	130
C2—H2B···O1^{i}	0.93	2.50	3.409 (3)	165
N1—H1A···O2^{i}	0.86	2.46	3.237 (2)	150
O3—H3···S1^{ii}	0.80	2.34	3.1361 (17)	177
C9—H9A···O2^{iii}	0.98	2.58	3.338 (2)	134

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*+1, *y*, *z*; (iii) −*x*+1/2, −*y*+2, *z*+1/2.

Fig. 1

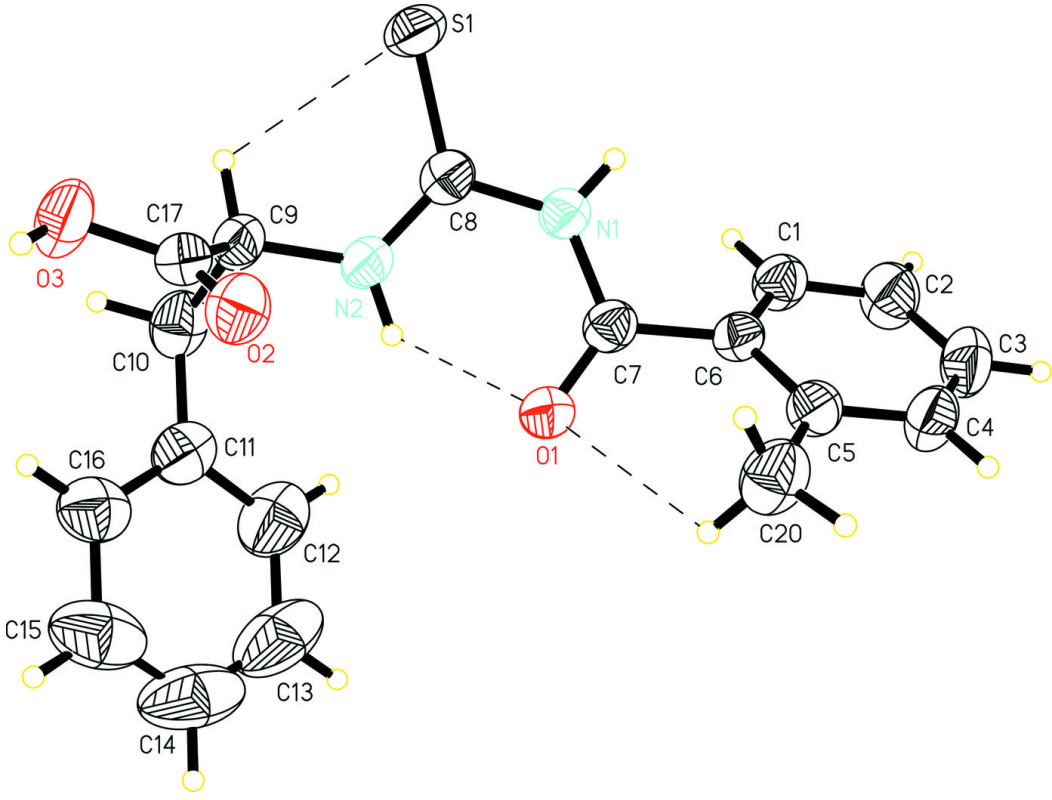
S1
C17
C9
C8
N1
C1
C2
O3
N2
C3
O2
C10
C7
C6
C4
O1
C5
C16
C11
C20
C12
C15
C13
C14

Fig. 2