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## Key indicators

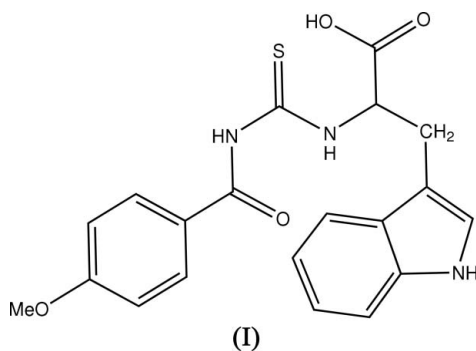
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.071  
 $wR$  factor = 0.139  
Data-to-parameter ratio = 13.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.3-(1*H*-Indol-3-yl)-2-[3-(4-methoxybenzoyl)-  
thioureido]propionic acid

In the title compound,  $\text{C}_{20}\text{H}_{19}\text{N}_3\text{O}_4\text{S}$ , the 3-methylene-1*H*-indole unit is nearly planar with a dihedral angle of  $2.69(2)^\circ$  between the rings. The crystal structure is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{N}-\text{H}\cdots\text{S}$ ,  $\text{O}-\text{H}\cdots\text{S}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming a two-dimensional network approximately parallel to the (011) plane.

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## Comment

The title compound, (I), is isostructural with 2-[3-(4-methoxybenzoyl)thioureido]-3-phenylpropionic acid methanol solvate, (II) (Ngah *et al.*, 2005). The molecule maintains the *cis-trans* configuration with respect to the positions of the 3-(1*H*-indole-3-yl)propionic acid and 4-methoxybenzoyl groups relative to the  $\text{C}=\text{S}$  bond across their  $\text{C}_9-\text{N}_2$  and  $\text{C}_9-\text{N}_1$  bonds, respectively (Fig. 1).



The  $\text{N}_3-\text{C}_{18}$  [1.360 (5)] and  $\text{N}_3-\text{C}_{19}$  [1.355 (5)  $\text{\AA}$ ] bonds in the indole ring system are slightly shorter than the corresponding ones [ $\text{N}_1-\text{C}_1 = 1.377$  (4) and  $\text{N}_1-\text{C}_8 = 1.369$  (4)  $\text{\AA}$ ] in 2-(2-acetamido-5-methylbenzoyl)-1*H*-indole (Ravishankar *et al.*, 2005). Other bond lengths and angles (Table 1) are in normal ranges (Allen *et al.*, 1987) and comparable to those in (II).

The central carbonylthiourea ( $\text{C}_8/\text{C}_9/\text{N}_1/\text{N}_2/\text{O}_2/\text{S}_1$ ) and 4-methoxyphenyl ( $\text{C}_1-\text{C}_6/\text{O}_1/\text{C}_7$ ) units are not planar with puckering amplitudes,  $Q_T$ , of 0.146 (1) and 0.143 (2)  $\text{\AA}$  (Cremer & Pople, 1975). Rings *A* ( $\text{C}_{12}/\text{C}_{13}/\text{C}_{18}/\text{N}_3/\text{C}_{19}$ ) and *B* ( $\text{C}_{13}-\text{C}_{18}$ ) in the 3-methylene-1*H*-indole system are each planar and they are nearly coplanar, with a dihedral angle of  $2.69(2)^\circ$ . Ring *A* has a pseudo-twofold axis running through  $\text{C}_{12}$  and the mid-point of the  $\text{N}_3-\text{C}_{18}$  bond (Table 1).

There are three intramolecular hydrogen bonds, viz.  $\text{N}_2-\text{H}_2\text{A}\cdots\text{O}_2$ ,  $\text{N}_2-\text{H}_2\text{A}\cdots\text{O}_3$  and  $\text{C}_{10}-\text{H}_{10}\cdots\text{S}_1$ , forming two pseudo-five-membered rings ( $\text{C}_{20}/\text{C}_{10}/\text{N}_2/\text{H}_2\text{A}/\text{O}_3$  and  $\text{C}_9/\text{N}_2/\text{C}_{10}/\text{H}_{10}/\text{S}_1$ ) and a pseudo-six-membered ring ( $\text{C}_8/\text{N}_1/\text{C}_9/\text{N}_2/\text{H}_2\text{A}/\text{O}_2$ ). The crystal structure is stabilized by inter-

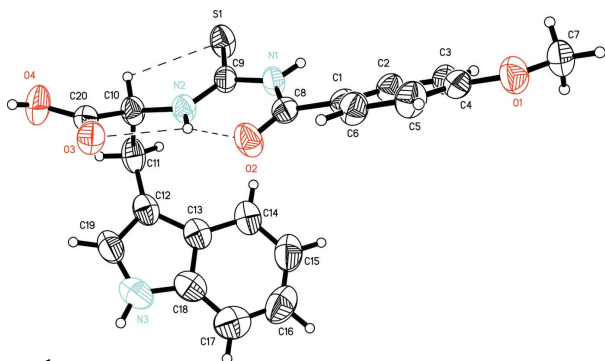


Figure 1

Molecular structure of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate intramolecular hydrogen bonds.

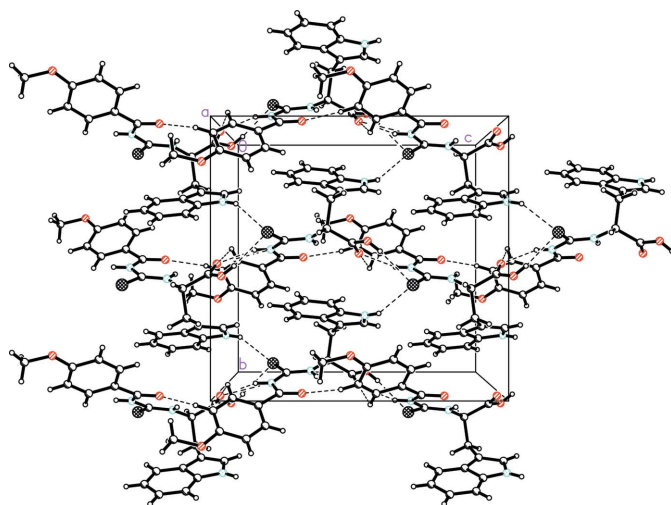


Figure 2

Packing diagram of (I), viewed down the *c* axis. Dashed lines denote intermolecular hydrogen bonds.

molecular hydrogen bonds (Table 2), forming a two-dimensional network approximately parallel to the (011) plane (Fig. 2).

## Experimental

Equimolar solutions of 4-methoxybenzoyl isothiocyanate (9.65 g, 0.05 mol) and DL-tryptophan (9.65 g, 0.05 mol) in acetone (50 ml) were mixed and refluxed for 5 h. The mixture was filtered into a beaker containing some ice cubes. The resulting brown precipitate was washed with cold acetone–distilled water before drying and kept in a desiccator (yield 15.4 g, 78%; m.p. 474.6–476.4 K). Recrystallization from chloroform yielded colorless single crystals suitable for X-ray analysis.

### Crystal data

$C_{20}H_{19}N_3O_4S$   
 $M_r = 397.44$   
 Orthorhombic, *Pbcn*  
 $a = 18.247$  (4) Å  
 $b = 14.083$  (3) Å  
 $c = 14.736$  (3) Å  
 $V = 3787.0$  (14) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.394$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 781 reflections  
 $\theta = 1.8$ – $25.0^\circ$   
 $\mu = 0.20$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, colorless  
 $0.19 \times 0.16 \times 0.15$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.962$ ,  $T_{\max} = 0.970$   
 18371 measured reflections

3343 independent reflections  
 2772 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$   
 $\theta_{\max} = 25.0^\circ$   
 $h = -21 \rightarrow 19$   
 $k = -13 \rightarrow 16$   
 $l = -17 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.071$   
 $wR(F^2) = 0.139$   
 $S = 1.26$   
 3343 reflections  
 255 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 2.2534P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.22$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

S1–C9	1.689 (3)	N1–C8	1.390 (4)
O2–C8	1.213 (3)	N2–C9	1.313 (4)
O3–C20	1.199 (4)	N2–C10	1.448 (4)
O4–C20	1.321 (4)	N3–C19	1.355 (5)
N1–C9	1.379 (4)	N3–C18	1.360 (5)
C9–N1–C8	127.6 (2)	N2–C9–N1	117.3 (3)
C9–N2–C10	123.8 (3)	N2–C9–S1	123.6 (2)
O2–C8–N1	121.8 (3)	N1–C9–S1	119.1 (2)
O2–C8–C1	122.6 (3)	N3–C18–C17	129.9 (4)
C19–C12–C13–C18	0.4 (4)	C13–C12–C19–N3	0.3 (4)
C19–N3–C18–C13	1.2 (4)	C18–N3–C19–C12	−0.9 (4)
C12–C13–C18–N3	−1.0 (4)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C10–H10...S1	0.98	2.64	3.059 (3)	106
N2–H2A...O2	0.86	1.95	2.628 (3)	135
N2–H2A...O3	0.86	2.37	2.680 (3)	102
N1–H1A...O3 <sup>i</sup>	0.86	2.13	2.955 (3)	160
N3–H3A...S1 <sup>ii</sup>	0.86	2.64	3.434 (3)	154
O4–H4...S1 <sup>iii</sup>	0.82	2.40	3.219 (3)	173
C2–H2...O3 <sup>i</sup>	0.93	2.44	2.986 (4)	118
C3–H3...O2 <sup>i</sup>	0.93	2.53	3.332 (4)	145

Symmetry codes: (i)  $x, -y + 2, z - \frac{1}{2}$ ; (ii)  $-x + \frac{3}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$ ; (iii)  $x, -y + 2, z + \frac{1}{2}$ .

H atoms were positioned geometrically, with O–H = 0.82 Å, N–H = 0.86 Å, and C–H = 0.93, 0.96, 0.97 and 0.98 Å for aromatic, methyl, methylene and methine H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{carrier atom})$ , where  $x = 1.5$  for methyl and hydroxyl H atoms, and  $x = 1.2$  for all other H atoms.

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

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