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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.079  
 $wR$  factor = 0.137  
Data-to-parameter ratio = 13.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.2-[3-(4-Methoxybenzoyl)thioureido]-3-  
phenylpropionic acid methanol solvate

In the title compound,  $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_4\text{S}\cdot\text{CH}_4\text{O}$ , the 4-methoxyphenyl and benzyl groups make dihedral angles of  $7.28$  ( $18$ ) and  $57.54$  ( $18$ ) $^\circ$ , respectively, with the central carbonylthiourea group. The crystal structure is stabilized by intermolecular hydrogen bonds,  $\text{N}-\text{H}\cdots\text{O}$ ,  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$ , forming a two-dimensional network parallel to the  $bc$  face.

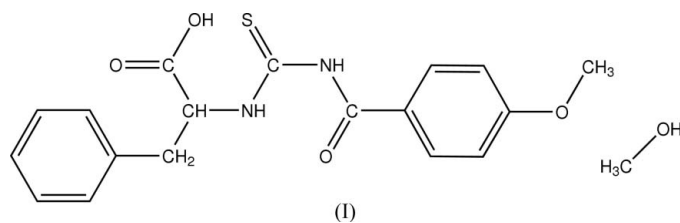
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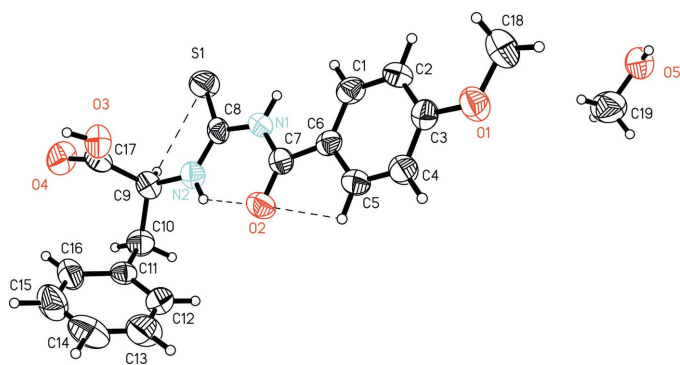
## Comment

The title compound, (I), is an amino acid derivative of thiourea and is isostructural with its analogues (2*S*)-2-(3-benzoylthioureido)-3-(1*H*)-imidazol-4-yl)propionic acid (Ngah, Shah, Yusof & Yamin, 2005) and (2*S*)-2-(3-benzoylthioureido)-3-methylbutyric acid (Ngah, Shah, Kassim & Yamin, 2005). However, the molecule is associated with one methanol molecule of crystallization (Fig. 1). The molecule maintains the *cis-trans* configuration with respect to the position of 3-phenylpropionic acid and 4-methoxybenzoyl groups relative to the  $\text{C}=\text{S}$  bond across their  $\text{C}8-\text{N}2$  and  $\text{C}8-\text{N}1$  bonds, respectively. Bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and comparable with those in the above-mentioned analogues (Yusof & Yamin, 2003; Ngah, Shah, Yusof & Yamin, 2005; Ngah, Shah, Kassim & Yamin, 2005).

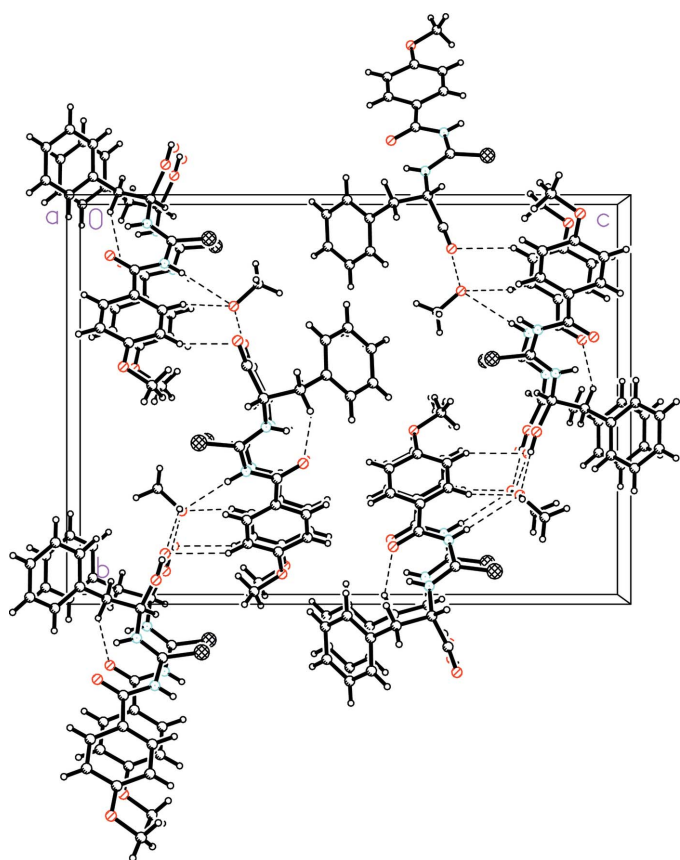


The 4-methoxyphenyl  $\text{C}1-\text{C}6/\text{O}1/\text{C}18$ , central carbonylthiourea  $\text{S}1/\text{O}2/\text{N}1/\text{N}2/\text{C}7/\text{C}8$  and benzyl  $\text{C}10/\text{C}11-\text{C}16$  groups are each planar. The maximum deviation is  $0.101$  ( $5$ ) Å for atom  $\text{C}18$  from the least-squares plane of the 4-methoxyphenyl group. The central carbonylthiourea fragment makes dihedral angles of  $7.28$  ( $18$ ) $^\circ$  and  $57.54$  ( $18$ ) $^\circ$  with the 4-methoxyphenyl and benzyl groups, respectively. The 4-methoxyphenyl and benzyl groups are inclined to each other by  $63.4$  ( $2$ ) $^\circ$ .

There are three intramolecular hydrogen bonds, *viz.*  $\text{C}5-\text{H}5\text{A}\cdots\text{O}2$ ,  $\text{C}9-\text{H}9\text{A}\cdots\text{S}1$  and  $\text{N}2-\text{H}2\text{A}\cdots\text{O}2$ , forming two pseudo-five-membered rings,  $\text{C}5/\text{H}5\text{A}/\text{O}2/\text{C}7/\text{C}6$  and  $\text{C}9/\text{H}9\text{A}/\text{S}1/\text{C}8/\text{N}2$ , and a pseudo-six-membered ring,  $\text{N}2/\text{H}2\text{A}/\text{O}2/\text{C}7/\text{N}1/\text{C}8$ . The crystal structure is stabilized by intermolecular hydrogen bonds (Table 2), forming a two dimensional network parallel to the  $bc$  face (Fig. 2).



**Figure 1**  
Molecular structure of (I), with 50% probability displacement ellipsoids. Dashed lines indicate the intramolecular hydrogen bonds.



**Figure 2**  
Packing diagram of (I), viewed down the *a* axis. Dashed lines denote O—H...O, N—H...O and C—H...O hydrogen bonds.

## Experimental

A solution of DL-phenylalanine in acetone was added dropwise to a two-necked round-bottomed flask containing an equimolar solution of 4-methoxybenzoyl isothiocyanate in acetone. The mixture was refluxed for about 5 h to complete the reaction, then filtered into a beaker containing some ice cubes. The white precipitate obtained was washed with cold acetone–distilled water before drying and kept in a desiccator (yield 81%; m.p. 449.3–453.1 K). Recrystallization from methanol yielded single crystals suitable for X-ray analysis.

## Crystal data

$C_{18}H_{18}N_2O_4S \cdot CH_4O$   
 $M_r = 390.45$   
 Orthorhombic,  $P2_12_12_1$   
 $a = 5.0364$  (13) Å  
 $b = 16.716$  (4) Å  
 $c = 23.040$  (6) Å  
 $V = 1939.7$  (8) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.337$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
 Cell parameters from 2510 reflections  
 $\theta = 1.5$ – $25.0^\circ$   
 $\mu = 0.20$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, colourless  
 $0.48 \times 0.19 \times 0.12$  mm

## Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.910$ ,  $T_{\max} = 0.976$   
 10023 measured reflections

3384 independent reflections  
 2977 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$   
 $\theta_{\max} = 25.0^\circ$   
 $h = -5 \rightarrow 5$   
 $k = -16 \rightarrow 19$   
 $l = -27 \rightarrow 27$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.079$   
 $wR(F^2) = 0.137$   
 $S = 1.33$   
 3384 reflections  
 257 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.7377P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.26$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.16$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 1384 Friedel pairs  
 Flack parameter: 0.03 (16)

**Table 1**

Selected bond lengths (Å).

S1—C8	1.660 (4)	O4—C17	1.196 (5)
O1—C3	1.364 (5)	N1—C7	1.382 (5)
O1—C18	1.419 (5)	N1—C8	1.394 (5)
O2—C7	1.210 (4)	N2—C8	1.320 (5)
O3—C17	1.312 (5)	N2—C9	1.446 (5)

**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>
N2—H2A...O2	0.86 (3)	1.96 (4)	2.630 (5)	134 (3)
C5—H5A...O2	0.93	2.47	2.784 (6)	100
C9—H9A...S1	0.98	2.72	3.052 (4)	100
N1—H1B...O5 <sup>i</sup>	0.85 (3)	2.53 (3)	3.358 (5)	164 (4)
O3—H3B...O5 <sup>ii</sup>	0.86 (3)	1.88 (3)	2.735 (5)	174 (6)
O5—H5B...O4 <sup>iii</sup>	0.85 (2)	2.26 (4)	2.789 (5)	121 (4)
C1—H1A...O5 <sup>i</sup>	0.93	2.49	3.377 (6)	161
C2—H2C...O4 <sup>iv</sup>	0.93	2.53	3.327 (5)	143
C10—H10B...O2 <sup>v</sup>	0.97	2.53	3.386 (6)	148
C13—H13A...O1 <sup>vi</sup>	0.93	2.60	3.488 (7)	160

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

H atoms attached to N and O atoms were located in a difference map and refined freely. Other H atoms were positioned geometrically in ideal positions after their location in a difference map, and allowed to ride on the parent (C) atom with C—H = 0.93–0.98 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for CH, CH<sub>2</sub>, and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub>.

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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