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1-(4-Chlorobenzoyl)-2-(1*H*-1,2,4-triazol-1-yl)-ethyl morpholine-4-carbodithioate

Zhi-Yi Wang,[a] Jun Wan,[b] Xue-Mei Li,[b] Chun-Li Li[b] and Shu-Sheng Zhang[b]*

[a]School of Materials and Environment Science, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 16.1

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

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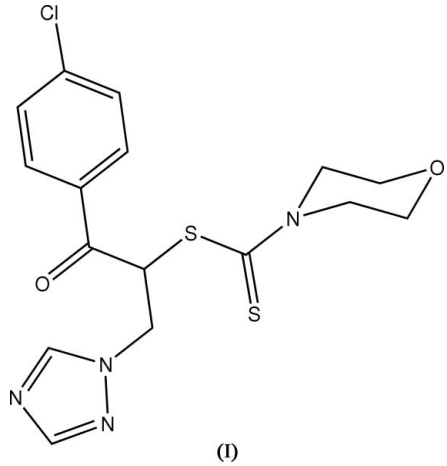
In the title compound, $C_{16}H_{17}ClN_4O_2S_2$, molecules are linked into chains along the *c* axis by C—H···O intermolecular interactions and further connected into a three-dimensional framework by other C—H···O interactions. The packing is stabilized by C—H···π and π–π interactions.

Comment

Many triazole compounds have good fungicidal and plant-growth-regulating activities (Xu *et al.*, 2002). Morpholine derivatives, an important type of fungicide, have attracted much interest because of their inward absorbent and broad-spectrum activities (Badioli *et al.*, 2001). In a search for new compounds with high bioactivity, the title compound, (I), was synthesized.



(I)

In the non-planar molecule, the orientation of the three rings is determined by the sp^3 hybridization state of atom C8. The two aromatic rings make a dihedral angle of 81.1 (1)°. The morpholine ring adopts a chair conformation.

In the crystal structure, molecules are linked into chains along the *c* axis *via* C—H···O hydrogen bonds (Fig. 2). The chains are further connected into a three-dimensional framework by other C—H···O interactions. The packing is stabilized by C—H···π (Table 2) and π–π interactions involving the benzene rings. The shortest distance between the centroids of neighbouring benzene rings is 3.700 (2) Å [$Cg\cdots Cg(-x, 1-y, 2-z)$ where *Cg* is the centroid of the triazole ring].

Experimental

The title compound was prepared according to a literature method (Wan *et al.*, 2005). Single crystals suitable for an X-ray diffraction

study were obtained by slow evaporation of an ethyl acetate–ethanol (1:3 *v*/*v*) solution over a period of one week.

Crystal data

$C_{16}H_{17}ClN_4O_2S_2$	D_x = 1.418 Mg m^{-3}
M_r = 396.91	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3432 reflections
a = 16.8253 (15) Å	θ = 2.4–24.1°
b = 7.4853 (7) Å	μ = 0.45 mm^{-1}
c = 14.8743 (13) Å	T = 293 (2) K
β = 97.171 (1)°	Block, pale yellow
V = 1858.7 (3) Å^3	0.26 × 0.19 × 0.05 mm
Z = 4	

Data collection

Siemens SMART 1K CCD area-detector diffractometer	3648 independent reflections
	2997 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.024
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.0°
	$h = -20 \rightarrow 20$
T_{min} = 0.893, T_{max} = 0.978	$k = -9 \rightarrow 9$
11068 measured reflections	$l = -18 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.6924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.108	
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
3648 reflections	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cl1—C3	1.738 (2)	O1—C7	1.208 (2)
S1—C12	1.781 (2)	C7—C8	1.537 (3)
S1—C8	1.819 (2)	C8—C9	1.522 (3)
S2—C12	1.661 (2)		
C9—C8—C7	113.15 (17)	C7—C8—S1	104.56 (14)
C9—C8—S1	108.31 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1^{i}	0.93	2.45	3.285 (3)	150
C9—H9A···O2^{ii}	0.97	2.53	3.412 (3)	150
C13—H13A···$Cg1^{i}$	0.97	2.89	3.656 (3)	137

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+1, -y, -z+2$. $Cg1$ is the centre of gravity for the triazole ring.

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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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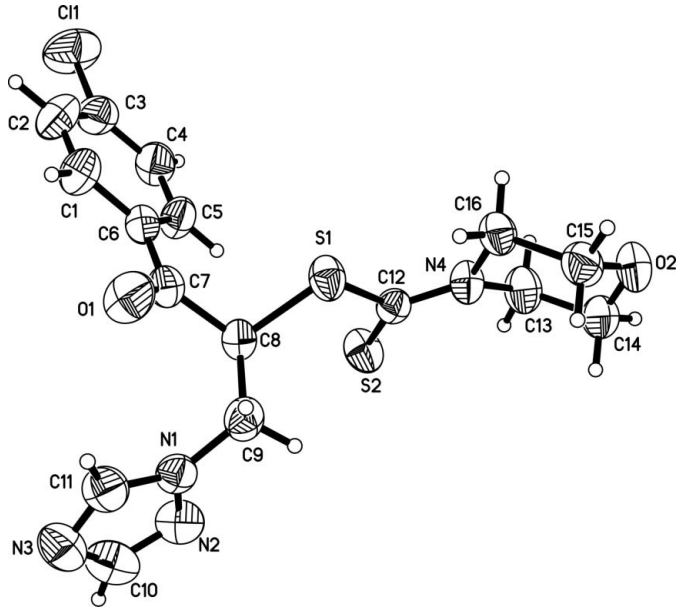

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

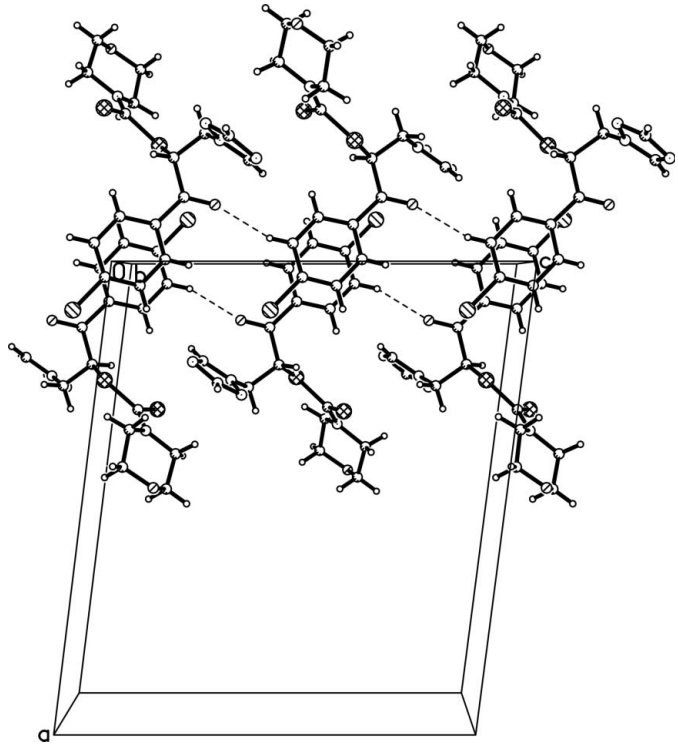

Figure 2
A view down the *b* axis, showing the chains along the *c* axis. Hydrogen bonds are indicated by dashed lines.

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