Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2,6-Dichlorophenyl)-3-(quinolin-2-yl)-thiazolidin-4-one

Resmi Raghunandan,[a] Ravindra K. Rawal,[b] S. B. Katti[b] and Prakas R. Maulik[a]*

[a]Molecular and Structural Biology Division, Central Drug Research Institute, Lucknow 226 001, India, and [b]Medicinal and Process Chemistry Division, Central Drug Research Institute, Lucknow 226 001, India

Correspondence e-mail: maulik_prakas@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 13.4

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

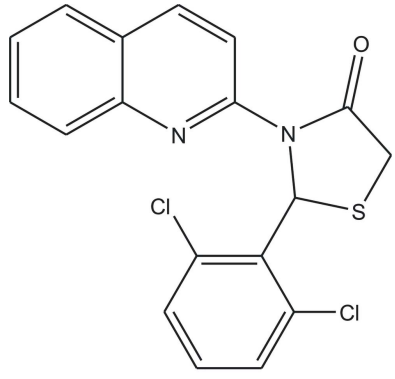
In the title molecule, $C_{18}H_{12}Cl_2N_2OS$, the thiazolidinone ring is planar and the quinoline and dichlorobenzene planes are twisted from it by 11.6 (1) and 85.2 (1)°, respectively. The crystal structure reveals the presence of π–π, C—H···O and C—H···Cl interactions, along with S···Cl short contacts.

Received 20 October 2006
Accepted 30 October 2006

CDRI communication No. 7061.

Comment

4-Thiazolidinones (Tanabe *et al.*, 1995) have many interesting biological activity profiles, for example as COX-1 inhibitors (Look *et al.*, 1996), inhibitors of the bacterial enzyme MurB (Anders *et al.*, 2001), non-nucleoside inhibitors of HIV–RT (Barreca *et al.*, 2001; Rawal *et al.* 2005) and antihistaminic agents (Diurno *et al.*, 1992). The therapeutic significance of thiazolidinone ring systems with suitably functionalized substituents has encouraged us to develop a novel synthesis in which different substituents could be arranged in a pharmacophoric pattern to display diverse pharmacological activities of higher orders (Rawal *et al.*, 2004; Srivastava *et al.*, 2002). Consequently, many different protocols have been developed that allow the synthesis of 4-thiazolidinone skeletons. These methods employ a one-pot three-component condensation or a two-step synthesis (Singh *et al.*, 1981). As not much is known about the exact binding site of this class of molecules, we thought it appropriate to obtain X-ray crystallographic data for a prototype. These data, especially regarding non-covalent interactions (Desiraju & Steiner, 1999), could be used for structural study and correlation. Hence the preparation and X-ray structure determination of the title compound, (I), was undertaken.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The central thiazolidinone ring is planar with an r.m.s. deviation of 0.025 Å. The quinoline and dichlorobenzene rings form dihedral angles of 11.6 (1) and 85.2 (1)°, respectively, with the

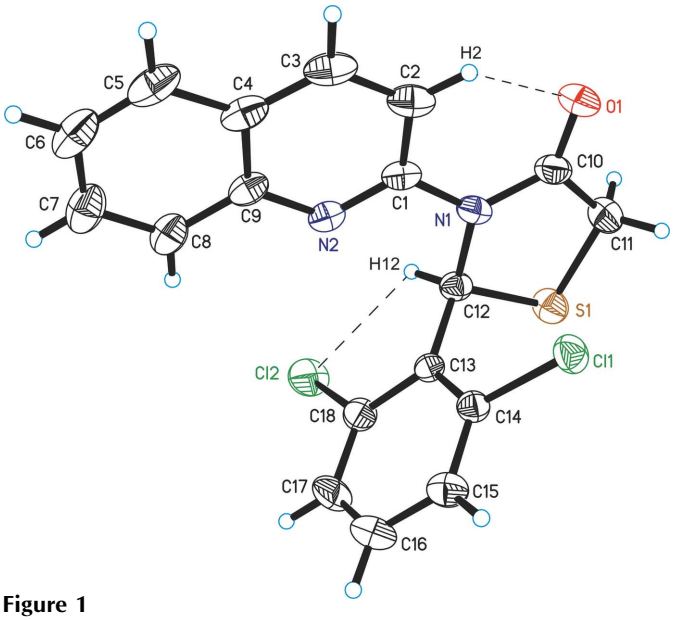


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacememt ellipsoids are drawn at the 30% probability level and dashed lines indicate hydrogen bonds.

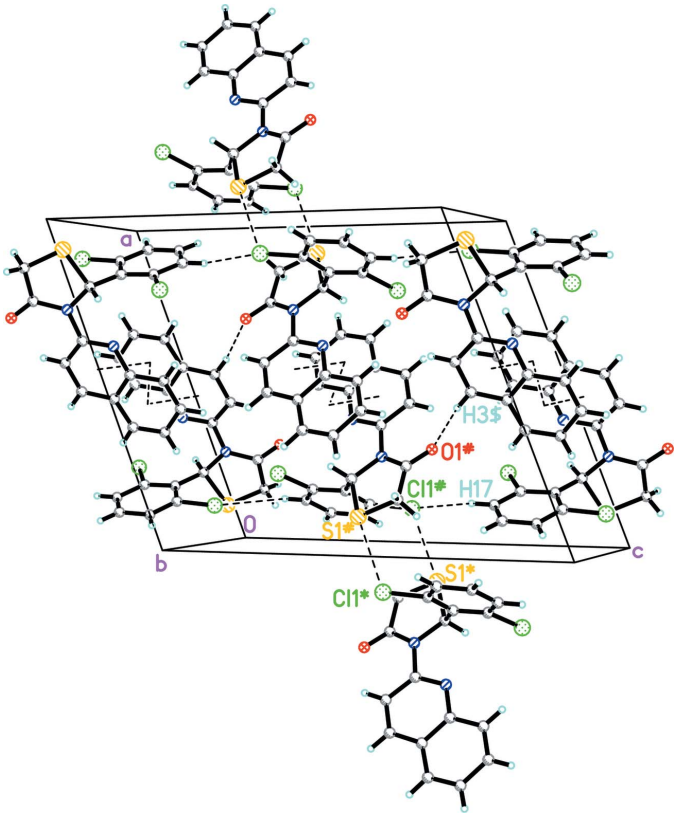


Figure 2
The crystal structure of (I). Dashed lines indicate intermolecular π–π, C—H···O, C—H···Cl and S···Cl interactions. Atoms labelled with the suffixes #, \$ and * are generated by the symmetry operations $(x, \frac{1}{2}-y, z-\frac{1}{2})$, $(1-x, 1-y, 2-z)$ and $(-x, \frac{1}{2}+y, \frac{3}{2}-z)$, respectively.

thiazolidinone ring. The crystal structure shows the presence of intermolecular π–π interactions (Meyer *et al.*, 2003) between the pyridine (centroid *Cg*1) and benzene rings (centroid *Cg*2) of the quinoline ring system, with *Cg*1···*Cg*2^{iii} and *Cg*2···*Cg*2^{iii} distances of 3.800 (2) and 3.606 (2) Å, respectively [symmetry code: (iii) $1-x, 1-y, 2-z$] (Fig. 2). The molecular packing is further stabilized by intermolecular C—H···O and C—H···Cl interactions (Table 1), along with an S1···Cl1($-x$, $-y$, $2-z$) short contact of 3.466 (1) Å (Fig. 2).

Experimental

Compound (I) was prepared from 2-aminoquinoline, 2,6-dichlorobenzaldehyde and mercaptoacetic acid according to a literature procedure (Srivastava *et al.*, 2002). Diffraction-quality crystals were grown by slow evaporation of an ethyl acetate–hexane (1:1 *v*/*v*) solution at room temperature.

Crystal data

$C_{18}H_{12}Cl_2N_2OS$
M_r = 375.26
Monoclinic, $P2_1/c$
a = 13.794 (1) Å
b = 7.868 (1) Å
c = 16.299 (2) Å
β = 111.36 (1)°
V = 1647.4 (3) Å^3
Z = 4
D_x = 1.513 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 293 (2) K
Block, colourless
0.28 × 0.25 × 0.23 mm

Data collection

Bruker P4 diffractometer
ω–2θ scans
Absorption correction: none
3812 measured reflections
2904 independent reflections
2053 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 25.0°
3 standard reflections
every 97 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 1.01
2904 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.216P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1	0.93	2.26	2.833 (4)	120
C3—H3···O1^{i}	0.93	2.56	3.468 (4)	167
C12—H12···Cl2	0.98	2.48	3.059 (3)	117
C17—H17···Cl1^{ii}	0.93	2.88	3.780 (3)	162

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

All H atoms were observable in the difference Fourier map. However, they were placed in idealized positions and allowed to ride on their parent C atoms, with C—H distances set at 0.97 (methylene), 0.93 (aromatic) or 0.98 Å (methine), and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 1997); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

RR thanks CSIR, India, for a Senior Research Fellowship.

References

Anders, C. J., Bronson, J. J., D'Andrea, S. V., Deshpande, S. M., Falk, P. J., Grant-Young, K. A., Harte, W. E., Ho, H., Misco, P. F., Robertson, J. G., Stock, D., Sun, Y. & Walsh, A. W. (2001). *Bioorg. Med. Chem. Lett.* **11**, 715–717.

Barreca, M. L., Chimirri, A., Luca, L. D., Monforte, A., Monforte, P., Rao, A., Zappala, M., Balzarini, J., De Clercq, E., Pannecouque, C. & Witvrouw, M. (2001). *Bioorg. Med. Chem. Lett.* **11**, 1793–1796.

Bruker (1997). *SHELXTL-NT*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Desiraju, G. R. & Steiner, T. (1999). *The Weak Hydrogen Bond in Structural Chemistry and Biology*. New York: Oxford University Press Inc.

Diurno, M. V., Mazzoni, O., Calignano, P. E., Giordano, F. & Bolognese, A. J. (1992). *J. Med. Chem.* **35**, 2910–2912.

Look, G. C., Schullek, J. R., Homes, C. P., Chinn, J. P., Gordon, E. M. & Gallop, M. A. (1996). *Bioorg. Med. Chem. Lett.* **6**, 707–712.

Meyer, E. A., Castellano, R. K. & Diederich, F. (2003). *Angew. Chem. Int. Ed.* **42**, 1210–1250.

Rawal, R. K., Prabhakar, Y. S., Katti, S. B. & Clercq, E. De. (2005). *Bioorg. Med. Chem.* **13**, 6771–6776.

Rawal, R. K., Srivastava, T., Haq, W. & Katti, S. B. (2004). *J. Chem. Res.* **5**, 368–369.

Siemens (1996). *XSCANS*. Version 2.21. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Singh, S. P., Parmar, S. S., Raman, K. & Stenberg, V. I. (1981). *Chem. Soc. Rev.* **81**, 175–203.

Srivastava, T., Haq, W. & Katti, S. B. (2002). *Tetrahedron*, **58**, 7619–7624.

Tanabe, Y., Yamamoto, H., Murakami, M., Yanagi, K., Kubota, Y., Okumura, H., Sanemitsu, Y. & Suzukamo, G. J. (1995). *J. Chem. Soc. Perkin Trans. 1*, pp. 935–947.