Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Chlorophenyl)-3-cyclohexylthiazolidin-4-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.119
Data-to-parameter ratio = 16.7

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

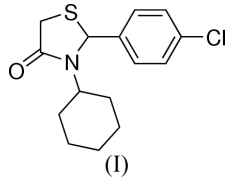
Received 16 July 2003
Accepted 25 July 2003
Online 31 July 2003

CDRI communication No. 6433.

The thiazolidine ring of the title molecule, $C_{15}H_{18}ClNOS$, is planar within 0.042 (3) Å and the cyclohexane ring adopts a chair conformation. The molecular structure is stabilized by weak C—H···O and C—H···π interactions. In the crystal structure, bifurcated C—H···O interactions link symmetry-related molecules to form dimers.

Comment

The therapeutic importance of suitably functionalized thiazolidinone ring systems (Anders *et al.*, 2001; Tanabe *et al.*, 1995; Diurno *et al.*, 1992) has encouraged us to develop an innovative synthesis in which different substituents could be arranged in a pharmacophoric pattern to display diverse pharmacological activities of higher order (Srivastava *et al.*, 2002). Since not much is known about the exact binding site of this class of molecules we thought it appropriate to generate X-ray crystal data of a prototype. Hence the X-ray structure determination of the title compound was undertaken. The data generated, especially 'non-covalent interactions' could be used for structural study and correlation. Non-covalent interactions play a significant role in molecular recognition, stabilization of DNA/RNA structures (Hobza & Sponer, 1999), crystal engineering (Desiraju, 1995) and drug development (Meyer *et al.*, 2003).



(I)

In the title molecule, (I) (Fig. 1), the central thiazolidinone ring is planar within 0.042 (3) Å and its conformation may be described as flattened envelope, with S1 deviating from the C2/N3/C4/C5 plane by 0.139 (1) Å. The cyclohexane ring adopts a chair conformation. The dihedral angle between the C2/N3/C4/C5 plane and the chlorophenyl ring is 83.5 (1)°. The molecular structure is stabilized by C—H···O and C—H···π interactions (Fig. 1 and Table 1). The crystal packing reveals that a molecule and its inversion equivalent are linked by bifurcated C—H···O interactions to form dimers (Fig. 2). The crystal structure is further stabilized by van der Waals interactions.

Experimental

The title compound was prepared from *p*-chlorobenzaldehyde and mercapotacetic acid, according to a literature procedure (Srivastava

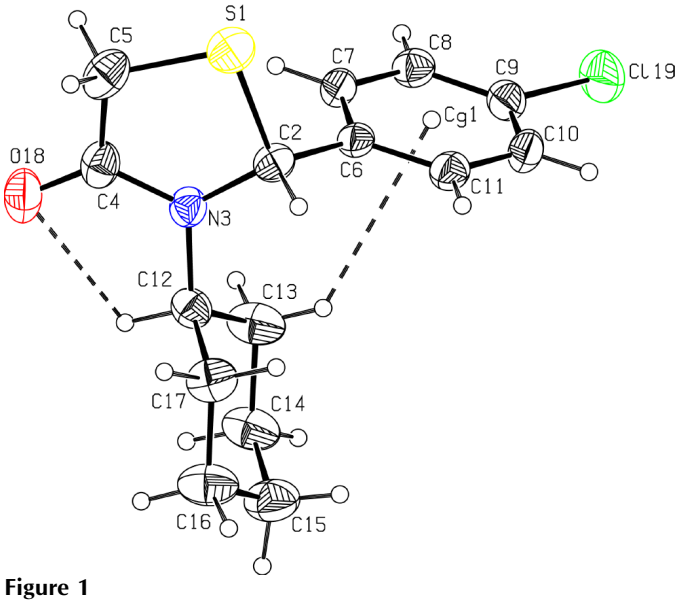


Figure 1
Displacement ellipsoid plot (30% probability), showing the molecular structure and the atom-labelling for the title compound. Non-covalent interactions are shown as dashed lines.

et al., 2002) and diffraction quality crystals were obtained by slow evaporation from a mixture of ethyl acetate and hexane (1:1).

Crystal data

$C_{15}H_{18}ClNOS$	D_x = 1.348 Mg m^{-3}
M_r = 295.81	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 40 reflections
a = 17.600 (1) Å	θ = 5.1–12.5°
b = 9.775 (1) Å	μ = 0.40 mm^{-1}
c = 17.089 (1) Å	T = 293 (2) K
β = 97.33 (1)°	Block, colourless
V = 2916.0 (4) Å^3	0.25 × 0.20 × 0.18 mm
Z = 8	

Data collection

Bruker $P4$ diffractometer	$h = -1 \rightarrow 21$
θ–2θ scans	$k = -1 \rightarrow 12$
Absorption correction: none	$l = -21 \rightarrow 20$
3556 measured reflections	3 standard reflections
2866 independent reflections	every 97 reflections
1731 reflections with $I > 2\sigma(I)$	frequency: 60 min
R_{int} = 0.023	intensity decay: none
θ_{max} = 26.0°	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 1.3546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.119	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
2866 reflections	
172 parameters	
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5B···O18^{i}	0.97	2.56	3.226 (4)	126
C7—H7···O18^{i}	0.93	2.68	3.601 (3)	169
C12—H12···O18	0.98	2.31	2.785 (3)	109
C13—H13A···Cg1	0.97	2.99	3.717 (3)	133

Symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} - y, -z$. Cg1 denotes the centroid of the substituted phenyl ring.

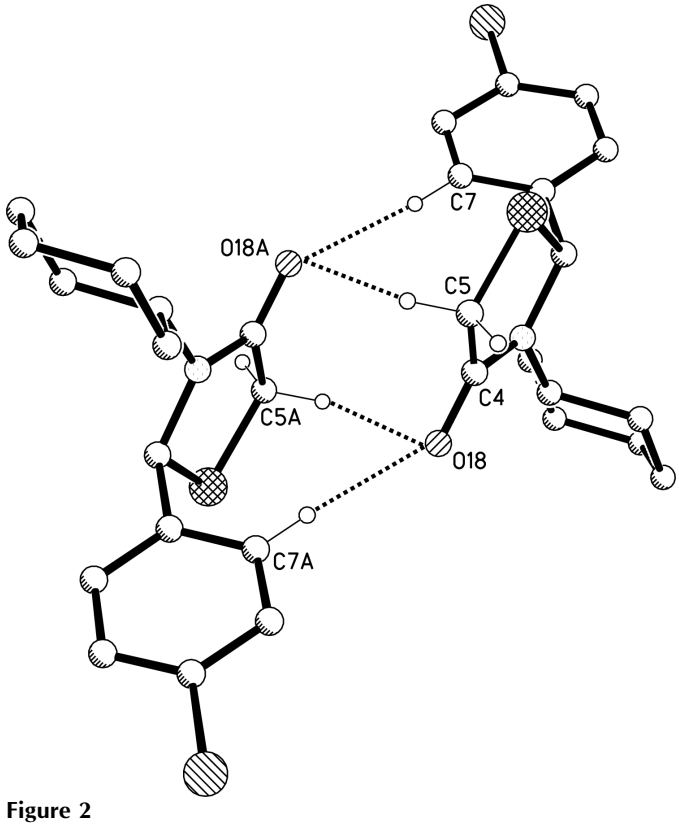


Figure 2
A view of the bifurcated C—H···O interactions leading to the formation of a dimer. Atoms labelled with the suffix A are at the symmetry position $(\frac{1}{2} - x, \frac{1}{2} - y, -z)$, *i.e.* symmetry code (i) in Table 1.

All H atoms were placed in calculated positions and allowed to ride on their parent C atoms, with C—H = 0.93–0.98 Å and 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* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

AS and TS thank CSIR, India, for providing Senior Research Fellowship.

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