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# 5-(4-Chlorophenoxy)-3,6-diphenyl-2-thioxo-2,3-dihydrothiazolo[4,5-*d*]pyrimidin-7(6*H*)-one 4-chlorophenol solvate

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**Key indicators**

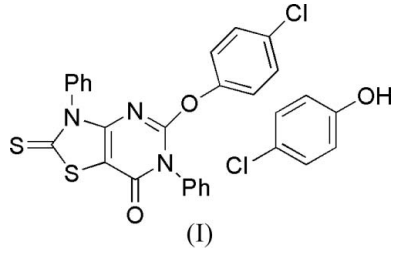
Single-crystal X-ray study
*T* = 292 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.048
*wR* factor = 0.140
Data-to-parameter ratio = 14.9

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

In the title compound, $C_{23}H_{14}ClN_3O_2S_2\cdot C_6H_5ClO$, the mean plane of the thiazolopyrimidine fragment makes dihedral angles of 64.26 (11), 77.70 (10) and 49.70 (18)° with the two attached phenyl rings and the 4-chlorophenoxy fragment. The crystal packing is stabilized by intermolecular O—H···O and intramolecular C—H···N hydrogen bonds, as well as by weak π–π stacking interactions.

## Comment

Thiazolo[4,5-*d*]pyrimidines can be considered as thia-analogues of the naturally occurring purine bases, adenine and guanine. These compounds have acquired a growing importance as anticancer immunotherapeutic agents (Nagahara *et al.*, 1990), antiviral agents used in the treatment of human cytomegalovirus (HCMV) (Revankar *et al.*, 1998), antitumour and antibacterial agents (Bekhit *et al.*, 2003; Fahmy *et al.*, 2003). In previous reports, an important synthetic route for these compounds has been the condensation reaction of 4-aminothiazole-5-carboxylate and isothiocyanate (Balkan *et al.*, 2002). However, this method often requires long reaction times. Recently, we have developed a versatile annulation process for the synthesis of novel thiazolo[4,5-*d*]pyrimidine derivatives. This process takes place smoothly under mild conditions, *via* a tandem aza-Wittig and cyclization reaction. In this paper, we report the structure of the title compound, (I) (Fig. 1).




(I)

In the molecule, all bond lengths and angles are normal (Allen *et al.*, 1987). The mean plane of the thiazolopyrimidine fragment makes dihedral angles of 64.26 (11), 77.70 (10) and 49.70 (18)°, respectively, with phenyl rings C1–C6 and C11–C16 and the 4-chlorophenoxy fragment. In the crystal structure, intermolecular O—H···O and intramolecular C—H···N hydrogen-bonding interactions stabilize the structure (Table 1). The crystal packing is further stabilized by weak π-π stacking interactions, as evidenced by the relatively short distances between the centroids of the N1/S2/C7–C9 (*Cg*1) and C18–C23 (*Cg*2) rings in adjacent molecules [$Cg1\cdots Cg1^{ii}$ = 3.8527 (13) Å and $Cg2\cdots Cg2^{iii}$ = 3.6018 (13) Å, symmetry codes: (ii) $-x, 2-y, 2-z$; (iii) $-x, 2-y, 1-z$].

## Experimental

The title compound was prepared according to the literature procedure of Liu *et al.* (2005). Suitable crystals of (I) were obtained by evaporation of a methanol solution (m.p. 509.4–510.6 K).

### *Crystal data*

$C_{23}H_{14}ClN_3O_2S_2\cdot C_6H_5ClO$
$M_r$ = 592.49
Triclinic, $P\overline{1}$
$a$ = 10.1348 (11) Å
$b$ = 11.5389 (13) Å
$c$ = 13.6575 (15) Å
$\alpha$ = 113.048 (2)°
$\beta$ = 95.896 (2)°
$\gamma$ = 105.972 (2)°
$V$ = 1372.4 (3) Å$^3$
$Z$ = 2
$D_x$ = 1.434 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.43 mm$^{-1}$
$T$ = 292 (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

### *Data collection*

Bruker SMART APEX CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
7829 measured reflections
5302 independent reflections
4250 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.071
$\theta_{max}$ = 26.0°

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
$S$ = 1.08
5302 reflections
356 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0761P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.45 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C23—H23···N2 | 0.93 | 2.55 | 2.893 (3) | 102 |
| O3—H3$A$···O1$^{i}$ | 0.83 (1) | 1.90 (2) | 2.681 (3) | 156 (4) |

Symmetry code: (i) $x, y, z-1$.

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with aromatic C—H = 0.93 Å and O—H = 0.83 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(O).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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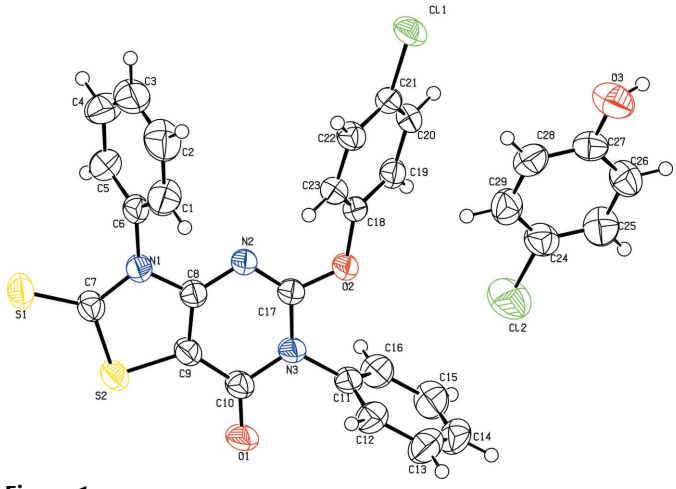


**Figure 1**
The molecular structure of (I), showing the labelling scheme and with displacement ellipsoids drawn at the 50% probability level.

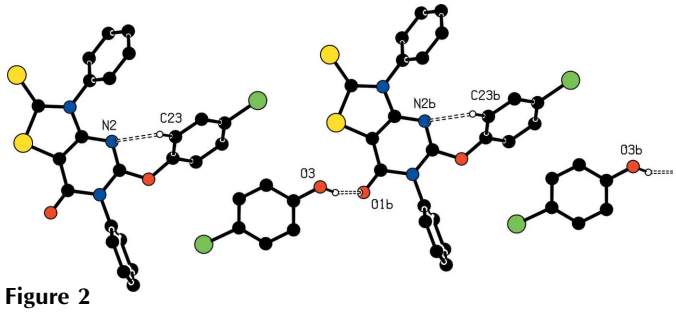


**Figure 2**
Part of the crystal structure of (I), showing the formation of O—H···O and C—H···N hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonds have been omitted. [Symmetry code: (b) $x, y, z-1$.]

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Balkan, A., Goren, Z. & Urgan, H. (2002). *Arzneim. Forsch.* **52**, 462–467.
Bekhit, A. A., Fahmy, H. T. Y., Rostom, S. A. F. & Baraka, A. M. (2003). *Eur. J. Med. Chem.* **38**, 27–32.
Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SMART* (Version 5.059) and *SAINT* (Version 6.01). Bruker AXS Inc., Madison, Wisconsin, USA.
Fahmy, H. T. Y., Rostom, S. A. F., Saudi, M. N. & Zjawiony, J. K. (2003). *Arch. Pharm. Pharm. Med. Chem.* **336**, 216–223.
Liu, J.-C., Chen, H.-L., Chen, T., He, H.-W. & Ding, M.-W. (2005). *Acta Cryst.* E**61**, o3187–o3189.
Nagahara, K., Anderson, J. D., Kini, G. D., Dalley, N. K., Larson, S. B., Smee, D. F., Jin, A., Sharma, B. S., Jolley, W. B. & Robins, R. K. (1990). *J. Med. Chem.* **33**, 407–415.
Revankar, G. R., Ojwang, J. O., Mustain, S. D., Rando, R. F., Clercq, E. D., Huffman, J. H., Drach, J. C., Sommadossi, J. P. & Lewis, A. F. (1998). *Antivir. Chem.* **9**, 53–63.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.