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3-[(2-Chlorothiazol-5-yl)methyl]-5-(isobutylamino)-6-phenyl-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7(6*H*)-one

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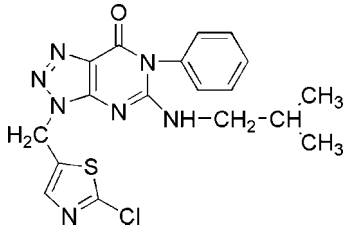
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.064; wR factor = 0.143; data-to-parameter ratio = 17.0.

The title compound, $C_{18}H_{18}ClN_7OS$, the mean plane of the triazolopyrimidine system makes dihedral angles of 77.54 (13) and 80.15 (13)°, respectively, with the attached phenyl and 2-chlorothiazole rings. The crystal packing is stabilized by intermolecular N—H···N hydrogen bonds and weak π–π stacking interactions [the interplanar distance is 3.724 (2) Å].

Related literature

For biological activities of 8-azapurines, see: Roblin *et al.* (1945); Shealy *et al.* (1984); Kidder *et al.* (1951); Lunt (1982). For the synthesis of triazolopyrimidine compounds, see: Ding *et al.* (2004); Wang *et al.* (2004).

For related literature, see: Sasada (1984); Wang *et al.* (1998).



Experimental

Crystal data

$C_{18}H_{18}ClN_7OS$
M_r = 415.90
Monoclinic, $C2/c$
a = 20.0916 (18) Å
b = 7.2538 (7) Å
c = 28.046 (2) Å
β = 101.527 (2)°
V = 4005.0 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 294 (2) K
0.20 × 0.10 × 0.04 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.939, T_{max} = 0.987
17095 measured reflections
4343 independent reflections
2226 reflections with $I > 2\sigma(I)$
R_{int} = 0.096

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.143
S = 0.98
4343 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7···N1^{i}	0.86	2.28	2.993 (4)	141

Symmetry code: (i) $x-\frac{1}{2}, y+\frac{1}{2}, z$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2311).

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supplementary materials

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3-[(2-Chlorothiazol-5-yl)methyl]-5-(isobutylamino)-6-phenyl-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7(6*H*)-one

L.-X. Xiao and D.-Q. Shi

Comment

8-aza analogues of similarly substituted purines ([1,2,3]triazolo[4,5-d]pyrimidines are one such example) have been synthesized in recent years, and many of them exhibit broad spectral biological activities, such as the interesting antifungal (Roblin *et al.*, 1945), antiviral (Shealy *et al.*, 1984), anticancer (Kidder *et al.*, 1951) and antiallergic (Lunt, 1982) activities. Recently, we have developed a versatile method via tandem aza-Wittig, followed by the cyclization to synthesize the novel triazolo[4,5-d]-pyrimidine derivatives (Ding *et al.*, 2004; Wang *et al.*, 2004). In this paper, we report the structure of the title compound, (I) (Fig. 1). In the triazolopyrimidine ring, the C5—N2, C5—N6, C6—N4, C7—N5 and C8—N5 bonds, Tabel 1, are significantly shorter than a normal single C—N bond (1.47Å ; Sasada, 1984) and closer to the value for a C═N bond (1.28 Å; Wang *et al.*, 1998). This indicates significant electron delocalization in the triazolo[4,5-d]pyrimidinyl system.

In the crystal structure, intermolecular N—H···N hydrogen-bonds contribute strongly to the stability of the molecular configuration (Fig.2 and Table 1). In addition, short intermolecular distances between the centroids of the C1–C2/N1/S1 ring (Cg1) and the C13–C18 ring (Cg4) of the adjacent molecule indicate the existence of weak π— π stacking interactions [Cg1···Cg4i =3.7237 (20) Å, dihedral angles of 5.94 (16)°, and a shortest interplanar distance of 3.388 Å.; symmetry code: (i) 1/2+x, -1/2+y, z.

Experimental

To a suspension of ethyl 1-((2-chlorothiazol-5-yl)methyl)- 5-((isobutylamino)(phenyl)methyleneamino)-1*H*-1,2,3-triazole-4-carboxylate (0.92 g, 2 mmol) in 10 ml of anhydrous ethanol, several drops of EtONa in EtOH were added at room temperature. The mixture was stirred for 10 min (monitored by thin layer chromatography), then the solution concentrated under vacuum and the residue was recrystallized from dichloromethane to give the title compound (yield 76%). Colourless crystals of (I) suitable for X-ray structure analysis were grown from a mixture of dichloromethane and ethanol (v/v, 1:3).

Refinement

All H atoms were placed in calculated positions, with C—H distances in the range 0.93-0.97 Å and N—H distances of 0.77-0.88 Å ,and included in the final cycles of refinement using a riding-model approximation, with $U_{iso}(H) = 1.2\text{-}1.5U_{eq}$(carrier atom).

Figures

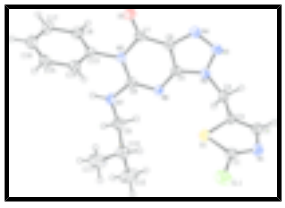

Fig. 1. The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

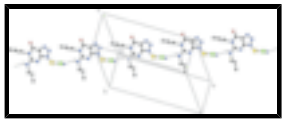

Fig. 2. Crystal packing diagram of (I). Hydrogen bonds are shown as dashed lines.

3-[(2-Chlorothiazol-5-yl)methyl]-5-(isobutylamino)-6-phenyl-3*H*- 1,2,3-triazolo[4,5-d]pyrimidin-7(6*H*)-one

Crystal data

$C_{18}H_{18}ClN_7OS$	F_{000} = 1728
M_r = 415.90	D_x = 1.380 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 1064 reflections
a = 20.0916 (18) Å	θ = 2.8–16.5º
b = 7.2538 (7) Å	μ = 0.32 mm^{-1}
c = 28.046 (2) Å	*T* = 294 (2) K
β = 101.527 (2)º	Block, colorless
V = 4005.0 (6) Å^3	0.20 × 0.10 × 0.04 mm
Z = 8	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	4343 independent reflections
Radiation source: fine-focus sealed tube	2226 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.096
T = 294(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 2001)	*h* = −25→25
T_{min} = 0.939, T_{max} = 0.987	*k* = −9→9
17095 measured reflections	*l* = −33→35

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$R[F^2 > 2\sigma(F^2)] = 0.064$

$wR(F^2) = 0.143$

$S = 0.98$

4343 reflections

255 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.28$ e Å^{-3}

$\Delta\rho_{min} = -0.25$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.45437 (18)	−0.1881 (5)	0.07899 (12)	0.0475 (9)
C2	0.49843 (16)	−0.1194 (5)	0.15347 (12)	0.0456 (9)
H2	0.5333	−0.1040	0.1805	0.055*
C3	0.43344 (15)	−0.0848 (4)	0.15564 (11)	0.0357 (8)
C4	0.40458 (15)	−0.0225 (5)	0.19814 (11)	0.0431 (9)
H4A	0.4402	−0.0224	0.2271	0.052*
H4B	0.3880	0.1027	0.1925	0.052*
C5	0.28245 (15)	−0.1132 (4)	0.19072 (10)	0.0331 (7)
C6	0.25197 (16)	−0.2612 (4)	0.20799 (11)	0.0383 (8)
C7	0.17957 (17)	−0.2757 (5)	0.19767 (11)	0.0387 (8)
C8	0.18729 (16)	0.0218 (4)	0.15449 (11)	0.0351 (8)
C9	0.18402 (17)	0.3310 (4)	0.11911 (13)	0.0482 (9)
H9A	0.2218	0.3564	0.1457	0.058*
H9B	0.1518	0.4312	0.1179	0.058*
C10	0.2099 (2)	0.3308 (6)	0.07249 (15)	0.0692 (12)
H10	0.2472	0.2415	0.0757	0.083*
C11	0.1566 (3)	0.2773 (7)	0.02910 (14)	0.1029 (17)
H11A	0.1441	0.1508	0.0321	0.154*
H11B	0.1743	0.2926	0.0000	0.154*
H11C	0.1174	0.3544	0.0275	0.154*
C12	0.2385 (2)	0.5219 (6)	0.06524 (18)	0.1065 (18)
H12A	0.2028	0.6118	0.0623	0.160*

H12B	0.2569	0.5222	0.0362	0.160*
H12C	0.2737	0.5517	0.0927	0.160*
C13	0.07716 (15)	−0.1286 (4)	0.15216 (11)	0.0341 (7)
C14	0.04907 (17)	−0.1883 (5)	0.10585 (11)	0.0461 (9)
H14	0.0768	−0.2274	0.0850	0.055*
C15	−0.02078 (19)	−0.1895 (5)	0.09071 (13)	0.0563 (10)
H15	−0.0401	−0.2282	0.0594	0.068*
C16	−0.06186 (18)	−0.1337 (5)	0.12179 (15)	0.0555 (10)
H16	−0.1088	−0.1348	0.1114	0.067*
C17	−0.03405 (18)	−0.0767 (5)	0.16788 (14)	0.0544 (10)
H17	−0.0621	−0.0401	0.1888	0.065*
C18	0.03624 (17)	−0.0733 (4)	0.18352 (12)	0.0446 (9)
H18	0.0554	−0.0341	0.2148	0.054*
Cl1	0.44869 (6)	−0.26117 (17)	0.02014 (3)	0.0838 (4)
N1	0.51130 (14)	−0.1786 (4)	0.10948 (10)	0.0489 (8)
N2	0.34916 (12)	−0.1415 (4)	0.20609 (9)	0.0375 (7)
N3	0.36005 (14)	−0.3031 (4)	0.23214 (9)	0.0474 (7)
N4	0.30135 (14)	−0.3749 (4)	0.23363 (9)	0.0488 (8)
N5	0.15024 (12)	−0.1259 (3)	0.16775 (8)	0.0361 (6)
N6	0.25402 (12)	0.0313 (4)	0.16422 (9)	0.0368 (7)
N7	0.15143 (13)	0.1615 (4)	0.13001 (9)	0.0426 (7)
H7	0.1082	0.1501	0.1206	0.051*
O1	0.14303 (12)	−0.3936 (3)	0.20981 (8)	0.0531 (7)
S1	0.38275 (4)	−0.12598 (13)	0.09935 (3)	0.0491 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.052 (2)	0.052 (2)	0.0397 (19)	0.0035 (19)	0.0133 (17)	−0.0012 (17)
C2	0.035 (2)	0.055 (2)	0.045 (2)	−0.0009 (18)	0.0037 (15)	−0.0014 (18)
C3	0.0272 (18)	0.042 (2)	0.0372 (18)	0.0041 (15)	0.0038 (14)	0.0002 (15)
C4	0.0303 (19)	0.056 (2)	0.044 (2)	−0.0006 (17)	0.0084 (15)	−0.0054 (17)
C5	0.0321 (18)	0.040 (2)	0.0281 (16)	0.0018 (16)	0.0090 (13)	−0.0037 (15)
C6	0.037 (2)	0.043 (2)	0.0369 (18)	0.0012 (17)	0.0103 (15)	0.0050 (16)
C7	0.042 (2)	0.044 (2)	0.0312 (17)	−0.0009 (18)	0.0085 (15)	0.0017 (16)
C8	0.0321 (19)	0.039 (2)	0.0348 (18)	0.0020 (16)	0.0086 (14)	0.0011 (15)
C9	0.041 (2)	0.033 (2)	0.068 (2)	0.0025 (16)	0.0060 (18)	0.0090 (18)
C10	0.062 (3)	0.068 (3)	0.080 (3)	−0.002 (2)	0.020 (2)	0.023 (2)
C11	0.114 (4)	0.131 (5)	0.061 (3)	−0.028 (3)	0.010 (3)	0.007 (3)
C12	0.106 (4)	0.087 (4)	0.138 (5)	−0.027 (3)	0.052 (3)	0.033 (3)
C13	0.0316 (18)	0.0351 (19)	0.0353 (18)	−0.0028 (15)	0.0061 (14)	0.0012 (15)
C14	0.043 (2)	0.055 (2)	0.0396 (19)	−0.0017 (18)	0.0068 (16)	−0.0028 (17)
C15	0.050 (2)	0.064 (3)	0.048 (2)	−0.009 (2)	−0.0092 (19)	0.005 (2)
C16	0.033 (2)	0.053 (2)	0.076 (3)	−0.0008 (19)	0.001 (2)	0.011 (2)
C17	0.040 (2)	0.053 (2)	0.074 (3)	−0.0021 (18)	0.022 (2)	−0.003 (2)
C18	0.042 (2)	0.051 (2)	0.0417 (19)	−0.0083 (17)	0.0088 (16)	−0.0063 (16)
Cl1	0.0986 (9)	0.1105 (10)	0.0437 (6)	0.0133 (7)	0.0175 (6)	−0.0084 (6)
N1	0.0382 (17)	0.060 (2)	0.0487 (18)	0.0021 (15)	0.0101 (14)	0.0000 (16)

N2	0.0318 (15)	0.0440 (17)	0.0366 (15)	0.0012 (13)	0.0068 (12)	0.0025 (13)
N3	0.0419 (18)	0.0529 (19)	0.0474 (17)	0.0120 (15)	0.0090 (14)	0.0155 (15)
N4	0.0411 (18)	0.0506 (19)	0.0550 (18)	0.0101 (15)	0.0105 (14)	0.0185 (15)
N5	0.0287 (14)	0.0424 (16)	0.0371 (15)	−0.0021 (13)	0.0064 (11)	0.0050 (13)
N6	0.0289 (16)	0.0404 (16)	0.0414 (15)	0.0008 (13)	0.0075 (12)	0.0079 (13)
N7	0.0259 (14)	0.0418 (17)	0.0584 (17)	−0.0007 (13)	0.0042 (13)	0.0138 (14)
O1	0.0468 (15)	0.0507 (16)	0.0617 (16)	−0.0091 (13)	0.0108 (12)	0.0176 (13)
S1	0.0348 (5)	0.0655 (7)	0.0443 (5)	0.0008 (5)	0.0014 (4)	−0.0024 (5)

Geometric parameters (Å, °)

C1—N1	1.286 (4)	C10—C11	1.503 (5)
C1—S1	1.711 (4)	C10—C12	1.529 (5)
C1—Cl1	1.715 (3)	C10—H10	0.9800
C2—C3	1.343 (4)	C11—H11A	0.9600
C2—N1	1.379 (4)	C11—H11B	0.9600
C2—H2	0.9300	C11—H11C	0.9600
C3—C4	1.496 (4)	C12—H12A	0.9600
C3—S1	1.725 (3)	C12—H12B	0.9600
C4—N2	1.460 (4)	C12—H12C	0.9600
C4—H4A	0.9700	C13—C18	1.378 (4)
C4—H4B	0.9700	C13—C14	1.378 (4)
C5—N2	1.339 (4)	C13—N5	1.446 (4)
C5—N6	1.344 (4)	C14—C15	1.383 (4)
C5—C6	1.372 (4)	C14—H14	0.9300
C6—N4	1.377 (4)	C15—C16	1.375 (5)
C6—C7	1.429 (4)	C15—H15	0.9300
C7—O1	1.219 (3)	C16—C17	1.366 (5)
C7—N5	1.426 (4)	C16—H16	0.9300
C8—N6	1.316 (4)	C17—C18	1.393 (4)
C8—N7	1.349 (4)	C17—H17	0.9300
C8—N5	1.397 (4)	C18—H18	0.9300
C9—N7	1.454 (4)	N2—N3	1.376 (3)
C9—C10	1.501 (5)	N3—N4	1.298 (3)
C9—H9A	0.9700	N7—H7	0.8600
C9—H9B	0.9700		
N1—C1—S1	117.4 (3)	C10—C11—H11C	109.5
N1—C1—Cl1	122.4 (3)	H11A—C11—H11C	109.5
S1—C1—Cl1	120.3 (2)	H11B—C11—H11C	109.5
C3—C2—N1	117.2 (3)	C10—C12—H12A	109.5
C3—C2—H2	121.4	C10—C12—H12B	109.5
N1—C2—H2	121.4	H12A—C12—H12B	109.5
C2—C3—C4	128.9 (3)	C10—C12—H12C	109.5
C2—C3—S1	109.1 (2)	H12A—C12—H12C	109.5
C4—C3—S1	122.0 (2)	H12B—C12—H12C	109.5
N2—C4—C3	111.8 (3)	C18—C13—C14	120.6 (3)
N2—C4—H4A	109.2	C18—C13—N5	120.2 (3)
C3—C4—H4A	109.2	C14—C13—N5	119.3 (3)
N2—C4—H4B	109.2	C13—C14—C15	119.4 (3)

C3—C4—H4B	109.2	C13—C14—H14	120.3
H4A—C4—H4B	107.9	C15—C14—H14	120.3
N2—C5—N6	125.8 (3)	C16—C15—C14	120.3 (3)
N2—C5—C6	104.8 (3)	C16—C15—H15	119.9
N6—C5—C6	129.4 (3)	C14—C15—H15	119.9
C5—C6—N4	109.1 (3)	C17—C16—C15	120.3 (3)
C5—C6—C7	119.6 (3)	C17—C16—H16	119.8
N4—C6—C7	131.3 (3)	C15—C16—H16	119.8
O1—C7—N5	119.8 (3)	C16—C17—C18	120.1 (3)
O1—C7—C6	129.8 (3)	C16—C17—H17	120.0
N5—C7—C6	110.3 (3)	C18—C17—H17	120.0
N6—C8—N7	119.0 (3)	C13—C18—C17	119.4 (3)
N6—C8—N5	124.1 (3)	C13—C18—H18	120.3
N7—C8—N5	116.9 (3)	C17—C18—H18	120.3
N7—C9—C10	115.6 (3)	C1—N1—C2	108.1 (3)
N7—C9—H9A	108.4	C5—N2—N3	110.1 (3)
C10—C9—H9A	108.4	C5—N2—C4	127.2 (3)
N7—C9—H9B	108.4	N3—N2—C4	122.6 (3)
C10—C9—H9B	108.4	N4—N3—N2	108.1 (2)
H9A—C9—H9B	107.4	N3—N4—C6	107.9 (3)
C9—C10—C11	113.0 (3)	C8—N5—C7	124.1 (3)
C9—C10—C12	108.6 (4)	C8—N5—C13	119.5 (2)
C11—C10—C12	110.6 (4)	C7—N5—C13	116.3 (2)
C9—C10—H10	108.2	C8—N6—C5	112.1 (3)
C11—C10—H10	108.2	C8—N7—C9	121.7 (3)
C12—C10—H10	108.2	C8—N7—H7	119.2
C10—C11—H11A	109.5	C9—N7—H7	119.2
C10—C11—H11B	109.5	C1—S1—C3	88.22 (16)
H11A—C11—H11B	109.5		
N1—C2—C3—C4	179.0 (3)	C3—C4—N2—N3	84.1 (3)
N1—C2—C3—S1	−0.4 (4)	C5—N2—N3—N4	−0.6 (3)
C2—C3—C4—N2	−127.6 (3)	C4—N2—N3—N4	178.7 (3)
S1—C3—C4—N2	51.7 (4)	N2—N3—N4—C6	0.7 (3)
N2—C5—C6—N4	0.3 (3)	C5—C6—N4—N3	−0.6 (4)
N6—C5—C6—N4	−179.7 (3)	C7—C6—N4—N3	179.1 (3)
N2—C5—C6—C7	−179.5 (3)	N6—C8—N5—C7	6.6 (5)
N6—C5—C6—C7	0.5 (5)	N7—C8—N5—C7	−173.7 (3)
C5—C6—C7—O1	−179.3 (3)	N6—C8—N5—C13	−175.5 (3)
N4—C6—C7—O1	1.0 (6)	N7—C8—N5—C13	4.2 (4)
C5—C6—C7—N5	2.1 (4)	O1—C7—N5—C8	175.8 (3)
N4—C6—C7—N5	−177.6 (3)	C6—C7—N5—C8	−5.5 (4)
N7—C9—C10—C11	53.4 (5)	O1—C7—N5—C13	−2.1 (4)
N7—C9—C10—C12	176.6 (3)	C6—C7—N5—C13	176.7 (3)
C18—C13—C14—C15	1.1 (5)	C18—C13—N5—C8	−98.9 (3)
N5—C13—C14—C15	−179.5 (3)	C14—C13—N5—C8	81.6 (4)
C13—C14—C15—C16	−0.8 (5)	C18—C13—N5—C7	79.0 (4)
C14—C15—C16—C17	0.0 (6)	C14—C13—N5—C7	−100.4 (3)
C15—C16—C17—C18	0.5 (5)	N7—C8—N6—C5	177.0 (3)
C14—C13—C18—C17	−0.5 (5)	N5—C8—N6—C5	−3.3 (4)

N5—C13—C18—C17	180.0 (3)	N2—C5—N6—C8	179.9 (3)
C16—C17—C18—C13	−0.3 (5)	C6—C5—N6—C8	−0.1 (4)
S1—C1—N1—C2	0.9 (4)	N6—C8—N7—C9	−7.2 (5)
Cl1—C1—N1—C2	−178.7 (3)	N5—C8—N7—C9	173.1 (3)
C3—C2—N1—C1	−0.3 (4)	C10—C9—N7—C8	88.0 (4)
N6—C5—N2—N3	−179.9 (3)	N1—C1—S1—C3	−1.0 (3)
C6—C5—N2—N3	0.2 (3)	Cl1—C1—S1—C3	178.6 (2)
N6—C5—N2—C4	0.9 (5)	C2—C3—S1—C1	0.7 (3)
C6—C5—N2—C4	−179.1 (3)	C4—C3—S1—C1	−178.8 (3)
C3—C4—N2—C5	−96.8 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7···N1^{i}	0.86	2.28	2.993 (4)	141

Symmetry codes: (i) *x*−1/2, *y*+1/2, *z*.

Fig. 1

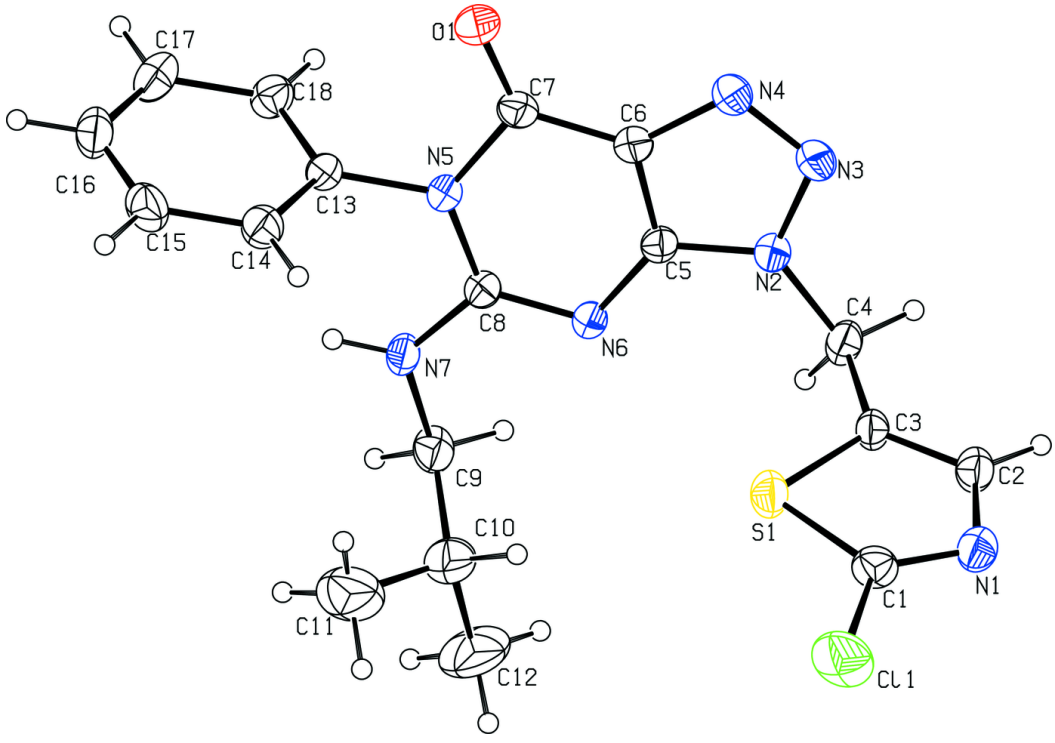
O1
C17
C18
C7
C6
N4
N5
N3
C16
C13
C15
C14
C5
N2
C8
N6
C4
N7
C3
C9
C2
S1
C10
N1
C1
C11
C12
Cl1

Fig. 2