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1-(Benzoylmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

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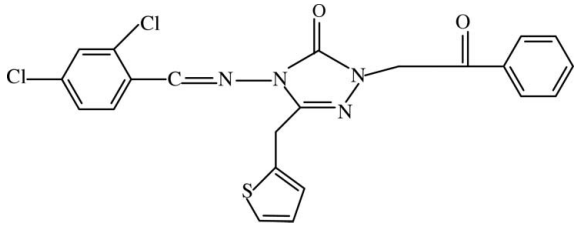
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in main residue; R factor = 0.049; wR factor = 0.131; data-to-parameter ratio = 16.8.

The thiophene ring of the title compound, $C_{22}H_{16}Cl_2N_4O_2S$, is disordered over two positions, corresponding to rotation of approximately 180° about the single C—C bond, with occupancies approximately in a 4:1 ratio. Weak C—H···O hydrogen bonds help in stabilizing the crystal structure.

Related literature

For related literature, see: Clemons *et al.* (2004); Ersan *et al.* (1998); Goss & Strasser-Weippl (2004); Holla *et al.* (1998, 2002); Liu *et al.* (1999); Palmer & Parsons (1996); Puviarasan *et al.* (1999); Sancak *et al.* (2005); Santen (2003); Tozkoparan *et al.* (2000); Turan-Zitouni, Kaplancikli, Erol & Kilic (1999); Vrábel *et al.* (2005); Yılmaz, Arslan, Kazak, Sancak & Er (2006); Zhu *et al.* (2000); Çoruh *et al.* (2003); İkizler *et al.* (1999).



Experimental

Crystal data

$C_{22}H_{16}Cl_2N_4O_2S$
M_r = 471.35
Orthorhombic, *Pbca*
a = 10.9045 (13) Å
b = 18.509 (2) Å
c = 21.228 (3) Å
V = 4284.4 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 293 (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
20905 measured reflections
5052 independent reflections
1671 reflections with $I > 2\sigma(I)$
R_{int} = 0.103

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.131
S = 0.84
5052 reflections
301 parameters
148 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 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
C21—H21···O21	0.93	2.23	2.916 (4)	130
C13—H13···O21^{i}	0.93	2.53	3.355 (7)	148

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2175).

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supplementary materials

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1-(Benzoylmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)-4,5-dihydro-1*H*-1,2,4-triazol-5-one

R. Ustabas, U. Çoruh, K. Sancak, Y. Ünver and E. M. Vázquez-López

Comment

1,2,4 triazole and 1,2,4 triazole-5-one derivatives have pharmacological properties as antimicrobial (Holla *et al.*, 1998; Ersan *et al.*, 1998; İkizler *et al.*, 1999), anti imflammatory, analgesic, antitumorial, antihypertensive, antiviral activities, coccidiostatic (Tozkoparan *et al.*, 2000; Turan-Zitouni *et al.*; 1999, Holla *et al.*, 2002). It was reported that compounds having triazole moieties such as Vorozole, Anastrozole and Letrozole appear to be very effective aromatase inhibitors very useful for preventing breast cancer (Goss *et al.*, 2004, Santen 2003, Clemons *et al.*, 2004). Spectroscopic and crystal structure data of some di-1,2,4-triazole-5-ones have been reported previously (Sancak *et al.*, 2005).

The compound was prepared and first identifed by NMR spectroscopy. In order to confirm the geometry, its X-ray structure determination was carried out. Compound (I) contains four planar rings (Fig. 1), namely two benzene rings [C22—C27 (A) and C33—C38 (B)], a triazole ring (C) and a thiophene ring (D). Deviations from the ideal bond-angle geometry around the Nsp^2 atoms of the single bond are observed. The N21—N2—C1 and N1—N3—C31 bond angles are 120.6 (3)° and 120.8 (3)°, respectively, too close to the ideal geometry (120°); however, the N21—N2—C2, C2—N3—C31 and N1—N3—C2 angles [130 (3)°, 124.5 (3)° and 114.1 (3)°, respectively] are distorted. In the triazole ring atom C2 deviate significantly from planarity. We can conclude, that the reason for these two deviation is intramolecular and intermolecular hydrogen bonds with the O21 atom.

The N21═C21 bond length [1.269 (4) Å] agree with values reported in the literature [1.261 (4) Å in the 4-amino-3-methtl-1,2,4-triazole- 5-thione derivative of *p*-nitrobenzaldehyde (Liu *et al.*, 1999), 1.267 (2) Å in 4-(4-hydroxybenzylidenamino)-4*H*-1,2,4-triazole hemihydrate (Zhu *et al.*, 2000) and 1.271 (3) Å in the 1-acetyl-4- (*p*-chlorobenzylideneamino)-3-methyl-4,5-dihydro-1*H*-1,2,4-triazol-5-one (Çoruh *et al.*, 2003)]. The presence of a substituent on N3 causes a lengthening of the N—N bond length [N1—N3= 1.385 (4) Å] with respect to the corresponding bonds in 5-(2-chlorophenyl)-4-phenyl-3,4-dihydro-2*H*-1,2,4-triazole-3-thione [N—N= 1.374 (2) Å; Puviarasan *et al.*, 1999] and in 4-methyl-1,2,4- triazole and 1-methyltetrazole [N—N= 1.344 (2) Å; Palmer & Parsons, 1996]. The S—C bond lengths [S11—C12= 1.692 (6) Å and S11—C15= 1.685 (5) Å] agree with value reported in the literature (Vrábel *et al.*, 2005; Yılmaz *et al.*, 2006)].

The thiophene ring is disordered over two positions, corresponding to rotation of approximately 180° about the single C11—C12 bond, with a major-minor ratio of about 78.5:21.5. Such flip-type disorder is rather common in thiophene rings. Weak C—H···O hydrogen bonds may help in stabilizing the crystal structure.

Experimental

3-thiophen-2-yl-methyl-4-aryliden amino-4,5-dihydro-1*H*-1,2,4-triazole-5-one (0.01 mol)was refluxed with an equivalent amount of natrium in absolute ethanol for 1 h. Then, ethyl bromoacetophenon (0.01 mol) was added and refluxed for an additional 5 h. The precipitate was filtered off, washed with H_2O and recrystallized from ethyl alcohol (yield: 72.47%) to give compound 1. m.p.421–422 °K.

IR (KBr) (v, cm^{-1}) 1698 (acetophenon-C=O), 1717 (triazole-C=O), 1584 (–C=N); ^{1}H NMR (DMSO-d6) δ (p.p.m.) 4.27 (s, thiophen-CH_2), 5.44 (s, –NCH_2), 6.95–7.06 (m, 2H, arH), 7.40–7.73 (m, 4H, arH), 7.81–8.15 (m, 4H, arH), 10.12 (s, –N=CH); ^{13}C NMR (DMSO-d6) δ (p.p.m.) 25.28 (thiophen-CH_2), 51.80 (–NCH_2), thiophen C:[125.42 (CH), 126.74 (CH), 126.86 (CH), 135.11(C)], ar C: [128.06 (CH), 129.56 (C), 135.11 (C), 136.72(C)], benzene C: [128.20 (CH), 128.83 (CH), 133.93 (C), 134.07 (CH)], 149.89 (triazole-C-5), 144.76 (triazole-C-3), 147.95 (–N=CH), 192.56 (acetophenon-C=O).

Refinement

The crystal was poor quality. All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) and 0.97 Å (methylene) and with U_{iso}(H) = 1.2U_{eq}(C).

Figures

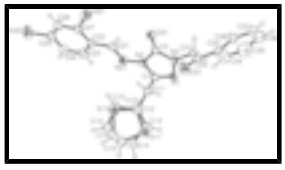


Fig. 1. An *ORTEP* drawing of (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

1-(benzoylmethyl)-4-[(2,4-dichlorobenzylidene)amino]-3-(2-thienylmethyl)- 4,5-dihydro-1*H*-1,2,4-triazol-5-one

Crystal data

$C_{22}H_{16}Cl_2N_4O_2S$	F_{000} = 1936
M_r = 471.35	D_x = 1.461 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 1671 reflections
a = 10.9045 (13) Å	θ = 1.9–28.0º
b = 18.509 (2) Å	μ = 0.43 mm^{-1}
c = 21.228 (3) Å	*T* = 293 (2) K
V = 4284.4 (9) $Å^3$	Prism, colourless
Z = 8	0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	1671 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.103
Monochromator: graphite	θ_{max} = 28.0º
T = 293(2) K	θ_{min} = 1.9º
φ and ω scans	*h* = −14→14
Absorption correction: none	*k* = −24→18
20905 measured reflections	*l* = −27→28
5052 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.84$	$(\Delta/\sigma)_{max} < 0.001$
5052 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
301 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
148 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Cl21	1.32634 (11)	0.05797 (7)	0.56626 (5)	0.0926 (4)	
Cl22	1.36468 (11)	−0.14685 (6)	0.39064 (6)	0.1026 (5)	
O21	1.0206 (2)	0.19915 (13)	0.60310 (11)	0.0607 (7)	
N21	0.9952 (3)	0.12711 (16)	0.47299 (13)	0.0509 (8)	
N2	0.9344 (2)	0.18406 (16)	0.50114 (13)	0.0480 (7)	
N1	0.7847 (3)	0.26329 (17)	0.50817 (15)	0.0605 (9)	
N3	0.8565 (3)	0.26362 (16)	0.56198 (14)	0.0570 (8)	
C21	1.0907 (3)	0.1034 (2)	0.50017 (17)	0.0525 (10)	
H21	1.1181	0.1249	0.5371	0.063*	
C22	1.1579 (3)	0.04203 (19)	0.47348 (17)	0.0465 (9)	
C2	0.9483 (3)	0.2137 (2)	0.56163 (18)	0.0497 (9)	
C26	1.3275 (4)	−0.0427 (2)	0.4762 (2)	0.0662 (11)	
H26	1.3978	−0.0599	0.4960	0.079*	
C27	1.2647 (3)	0.0163 (2)	0.50036 (17)	0.0547 (10)	
C33	0.8744 (3)	0.4183 (2)	0.68112 (18)	0.0543 (10)	
C1	0.8337 (3)	0.2147 (2)	0.47287 (17)	0.0533 (10)	
C31	0.8221 (3)	0.30610 (19)	0.61592 (15)	0.0547 (10)	

H31A	0.8254	0.2758	0.6532	0.066*	
H31B	0.7380	0.3221	0.6107	0.066*	
C32	0.9029 (3)	0.3716 (2)	0.62635 (18)	0.0531 (10)	
O31	0.9870 (3)	0.38367 (15)	0.59117 (14)	0.0891 (10)	
C11	0.7843 (3)	0.1924 (2)	0.41043 (16)	0.0578 (9)	
H11A	0.6975	0.2038	0.4091	0.069*	
H11B	0.7922	0.1404	0.4066	0.069*	
C12	0.8453 (5)	0.2270 (3)	0.3550 (2)	0.0571 (9)	0.785 (3)
S11	0.98134 (13)	0.19883 (9)	0.32561 (8)	0.0713 (6)	0.785 (3)
C13	0.7886 (6)	0.2802 (4)	0.3212 (3)	0.0666 (12)	0.785 (3)
H13	0.7121	0.3004	0.3294	0.080*	0.785 (3)
C14	0.8751 (5)	0.3000 (3)	0.2677 (3)	0.0716 (11)	0.785 (3)
H14	0.8590	0.3364	0.2387	0.086*	0.785 (3)
C15	0.9759 (5)	0.2598 (3)	0.2667 (3)	0.0725 (12)	0.785 (3)
H15	1.0372	0.2647	0.2366	0.087*	0.785 (3)
C12'	0.8527 (12)	0.2212 (7)	0.3532 (3)	0.0616 (14)*	0.215 (3)
S11'	0.8163 (7)	0.2950 (4)	0.3095 (4)	0.0722 (14)*	0.215 (3)
C13'	0.9566 (14)	0.1860 (9)	0.3320 (8)	0.0663 (19)*	0.215 (3)
H13'	0.9914	0.1447	0.3495	0.080*	0.215 (3)
C14'	1.0039 (14)	0.2273 (9)	0.2747 (8)	0.0687 (19)*	0.215 (3)
H14'	1.0734	0.2137	0.2522	0.082*	0.215 (3)
C15'	0.9356 (11)	0.2849 (8)	0.2600 (6)	0.068 (2)*	0.215 (3)
H15'	0.9521	0.3157	0.2265	0.081*	0.215 (3)
C24	1.1791 (4)	−0.0510 (2)	0.3943 (2)	0.0761 (12)	
H24	1.1499	−0.0739	0.3583	0.091*	
C38	0.7842 (4)	0.4019 (2)	0.72463 (19)	0.0665 (11)	
H38	0.7378	0.3601	0.7198	0.080*	
C25	1.2842 (4)	−0.0750 (2)	0.4228 (2)	0.0667 (12)	
C23	1.1168 (3)	0.0070 (2)	0.41901 (19)	0.0625 (11)	
H23	1.0460	0.0232	0.3992	0.075*	
C37	0.7628 (5)	0.4467 (3)	0.7749 (2)	0.0892 (14)	
H37	0.7013	0.4354	0.8036	0.107*	
C35	0.9191 (6)	0.5250 (3)	0.7406 (3)	0.1083 (18)	
H35	0.9649	0.5669	0.7460	0.130*	
C34	0.9415 (4)	0.4808 (3)	0.6892 (2)	0.0797 (13)	
H34	1.0017	0.4932	0.6601	0.096*	
C36	0.8312 (6)	0.5078 (3)	0.7831 (3)	0.1050 (18)	
H36	0.8175	0.5374	0.8178	0.126*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl21	0.0910 (9)	0.1162 (10)	0.0705 (8)	0.0339 (7)	−0.0225 (7)	−0.0168 (7)
Cl22	0.1150 (10)	0.0628 (7)	0.1300 (11)	0.0048 (7)	0.0437 (8)	−0.0204 (7)
O21	0.0489 (15)	0.0879 (19)	0.0453 (16)	0.0102 (14)	−0.0114 (13)	−0.0059 (14)
N21	0.046 (2)	0.061 (2)	0.0453 (19)	−0.0011 (17)	−0.0025 (17)	−0.0016 (16)
N2	0.0382 (17)	0.065 (2)	0.040 (2)	0.0063 (16)	−0.0019 (16)	−0.0020 (16)
N1	0.056 (2)	0.087 (2)	0.039 (2)	0.0132 (18)	−0.0074 (17)	0.0020 (17)

N3	0.0498 (19)	0.080 (2)	0.042 (2)	0.0140 (18)	0.0010 (16)	−0.0066 (17)
C21	0.048 (2)	0.063 (3)	0.047 (2)	−0.008 (2)	0.001 (2)	−0.002 (2)
C22	0.045 (2)	0.052 (2)	0.043 (2)	−0.008 (2)	0.0049 (19)	0.0014 (19)
C2	0.037 (2)	0.068 (3)	0.044 (2)	0.002 (2)	0.0044 (19)	0.002 (2)
C26	0.063 (3)	0.059 (3)	0.076 (3)	0.005 (2)	0.013 (2)	0.006 (2)
C27	0.062 (3)	0.059 (3)	0.044 (2)	−0.001 (2)	0.004 (2)	0.002 (2)
C33	0.048 (2)	0.055 (3)	0.060 (3)	0.009 (2)	−0.003 (2)	0.008 (2)
C1	0.042 (2)	0.073 (3)	0.044 (2)	0.000 (2)	0.002 (2)	0.004 (2)
C31	0.051 (2)	0.069 (3)	0.044 (2)	0.013 (2)	0.0054 (18)	0.003 (2)
C32	0.047 (3)	0.061 (3)	0.052 (3)	0.006 (2)	0.002 (2)	0.011 (2)
O31	0.081 (2)	0.095 (2)	0.092 (2)	−0.0135 (17)	0.0432 (19)	0.0022 (17)
C11	0.0467 (19)	0.074 (2)	0.053 (2)	−0.0016 (18)	−0.0051 (16)	0.0004 (17)
C12	0.0515 (17)	0.0686 (19)	0.0513 (18)	−0.0075 (16)	−0.0054 (15)	−0.0050 (16)
S11	0.0475 (8)	0.1012 (12)	0.0653 (10)	−0.0089 (8)	0.0079 (7)	−0.0066 (9)
C13	0.064 (2)	0.075 (2)	0.061 (2)	−0.013 (2)	0.000 (2)	0.0037 (19)
C14	0.077 (2)	0.080 (2)	0.058 (2)	−0.014 (2)	−0.001 (2)	0.0063 (19)
C15	0.069 (2)	0.088 (2)	0.061 (2)	−0.018 (2)	0.0086 (19)	−0.004 (2)
C24	0.083 (3)	0.070 (3)	0.075 (3)	−0.018 (3)	0.010 (3)	−0.012 (3)
C38	0.064 (3)	0.073 (3)	0.063 (3)	0.012 (2)	0.006 (2)	0.001 (2)
C25	0.077 (3)	0.046 (3)	0.077 (3)	−0.002 (2)	0.028 (3)	−0.005 (2)
C23	0.058 (3)	0.064 (3)	0.066 (3)	−0.006 (2)	0.005 (2)	−0.002 (2)
C37	0.105 (4)	0.093 (4)	0.070 (3)	0.031 (3)	0.016 (3)	−0.009 (3)
C35	0.138 (5)	0.075 (4)	0.112 (5)	−0.016 (4)	−0.025 (4)	−0.022 (4)
C34	0.069 (3)	0.079 (4)	0.091 (4)	−0.010 (3)	0.000 (3)	0.003 (3)
C36	0.146 (5)	0.085 (4)	0.084 (4)	0.032 (4)	−0.004 (4)	−0.017 (3)

Geometric parameters (Å, °)

Cl21—C27	1.733 (4)	C12—C13	1.367 (8)
Cl22—C25	1.733 (4)	C12—S11	1.692 (6)
O21—C2	1.212 (4)	S11—C15	1.685 (5)
N21—C21	1.269 (4)	C13—C14	1.522 (9)
N21—N2	1.381 (4)	C13—H13	0.9300
N2—C1	1.374 (4)	C14—C15	1.328 (6)
N2—C2	1.405 (4)	C14—H14	0.9300
N1—C1	1.287 (4)	C15—H15	0.9300
N1—N3	1.385 (4)	C12'—C13'	1.383 (13)
N3—C2	1.362 (4)	C12'—S11'	1.698 (12)
N3—C31	1.439 (4)	S11'—C15'	1.682 (10)
C21—C22	1.465 (5)	C13'—C14'	1.526 (12)
C21—H21	0.9300	C13'—H13'	0.9300
C22—C27	1.381 (4)	C14'—C15'	1.337 (11)
C22—C23	1.399 (5)	C14'—H14'	0.9300
C26—C25	1.367 (5)	C15'—H15'	0.9300
C26—C27	1.387 (5)	C24—C25	1.370 (5)
C26—H26	0.9300	C24—C23	1.374 (5)
C33—C34	1.378 (5)	C24—H24	0.9300
C33—C38	1.383 (5)	C38—C37	1.372 (5)
C33—C32	1.482 (5)	C38—H38	0.9300

C1—C11	1.489 (5)	C23—H23	0.9300
C31—C32	1.516 (5)	C37—C36	1.366 (6)
C31—H31A	0.9700	C37—H37	0.9300
C31—H31B	0.9700	C35—C36	1.355 (7)
C32—O31	1.204 (4)	C35—C34	1.386 (6)
C11—C12	1.495 (5)	C35—H35	0.9300
C11—C12'	1.522 (8)	C34—H34	0.9300
C11—H11A	0.9700	C36—H36	0.9300
C11—H11B	0.9700		
C21—N21—N2	117.5 (3)	C11—C12—S11	123.3 (5)
C1—N2—N21	120.6 (3)	C15—S11—C12	92.1 (3)
C1—N2—C2	108.9 (3)	C12—C13—C14	106.6 (5)
N21—N2—C2	130.0 (3)	C12—C13—H13	126.7
C1—N1—N3	104.4 (3)	C14—C13—H13	126.7
C2—N3—N1	114.1 (3)	C15—C14—C13	112.9 (5)
C2—N3—C31	124.5 (3)	C15—C14—H14	123.5
N1—N3—C31	120.8 (3)	C13—C14—H14	123.5
N21—C21—C22	120.2 (3)	C14—C15—S11	113.1 (4)
N21—C21—H21	119.9	C14—C15—H15	123.4
C22—C21—H21	119.9	S11—C15—H15	123.4
C27—C22—C23	116.8 (3)	C13'—C12'—C11	119.7 (12)
C27—C22—C21	121.9 (3)	C13'—C12'—S11'	113.1 (8)
C23—C22—C21	121.2 (4)	C11—C12'—S11'	127.1 (11)
O21—C2—N3	128.7 (4)	C15'—S11'—C12'	94.1 (6)
O21—C2—N2	130.3 (3)	C12'—C13'—C14'	107.5 (10)
N3—C2—N2	101.0 (3)	C12'—C13'—H13'	126.3
C25—C26—C27	118.7 (4)	C14'—C13'—H13'	126.3
C25—C26—H26	120.7	C15'—C14'—C13'	113.4 (11)
C27—C26—H26	120.7	C15'—C14'—H14'	123.3
C22—C27—C26	122.4 (4)	C13'—C14'—H14'	123.3
C22—C27—Cl21	120.5 (3)	C14'—C15'—S11'	112.0 (9)
C26—C27—Cl21	117.1 (3)	C14'—C15'—H15'	124.0
C34—C33—C38	118.7 (4)	S11'—C15'—H15'	124.0
C34—C33—C32	118.4 (4)	C25—C24—C23	119.9 (4)
C38—C33—C32	123.0 (4)	C25—C24—H24	120.1
N1—C1—N2	111.5 (3)	C23—C24—H24	120.1
N1—C1—C11	124.2 (3)	C37—C38—C33	120.5 (4)
N2—C1—C11	124.3 (4)	C37—C38—H38	119.8
N3—C31—C32	113.7 (3)	C33—C38—H38	119.8
N3—C31—H31A	108.8	C26—C25—C24	120.9 (4)
C32—C31—H31A	108.8	C26—C25—Cl22	119.1 (4)
N3—C31—H31B	108.8	C24—C25—Cl22	119.9 (4)
C32—C31—H31B	108.8	C24—C23—C22	121.3 (4)
H31A—C31—H31B	107.7	C24—C23—H23	119.3
O31—C32—C33	122.6 (4)	C22—C23—H23	119.3
O31—C32—C31	120.0 (3)	C36—C37—C38	120.5 (5)
C33—C32—C31	117.4 (3)	C36—C37—H37	119.8
C1—C11—C12	114.9 (3)	C38—C37—H37	119.8
C1—C11—C12'	115.8 (3)	C36—C35—C34	120.7 (5)

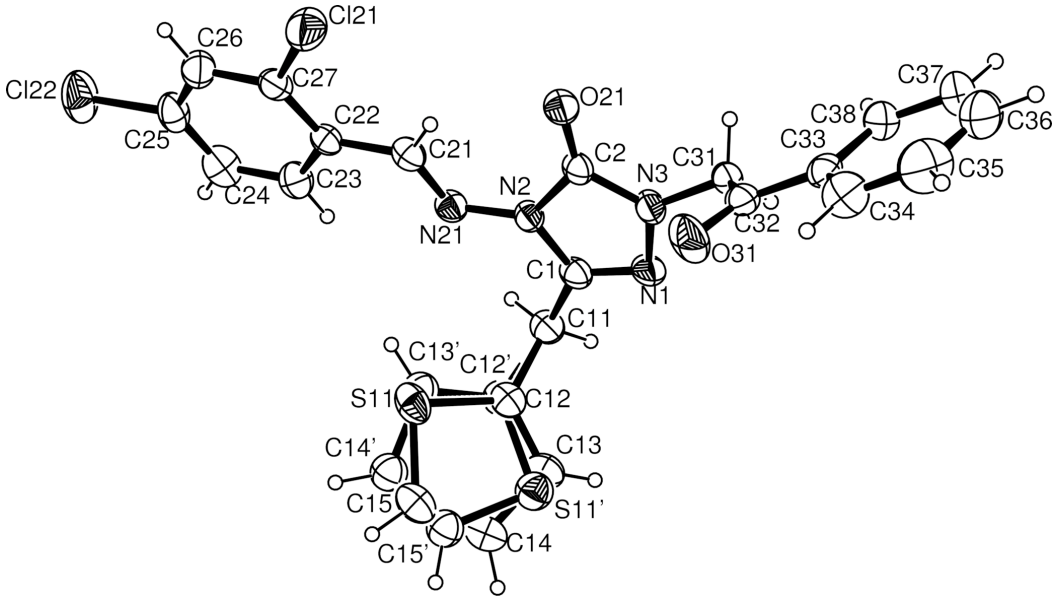
C1—C11—H11A	108.6	C36—C35—H35	119.6
C12—C11—H11A	108.6	C34—C35—H35	119.6
C12'—C11—H11A	112.3	C33—C34—C35	119.9 (5)
C1—C11—H11B	108.6	C33—C34—H34	120.0
C12—C11—H11B	108.6	C35—C34—H34	120.0
C12'—C11—H11B	103.7	C35—C36—C37	119.7 (5)
H11A—C11—H11B	107.5	C35—C36—H36	120.2
C13—C12—C11	121.4 (5)	C37—C36—H36	120.2
C13—C12—S11	115.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O21	0.93	2.23	2.916 (4)	130
C13—H13···O21^{i}	0.93	2.53	3.355 (7)	148

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

Fig. 1


Cl21
C26
Cl22
C27
C22
C25
C21
O21
C2
C23
C24
N2
N3
C31
C37
C38
C33
C36
C35
C34
N21
C32
O31
C1
N1
C11
C13'
C12'
S11
C12
C14'
C13
C15
S11'
C15'
C14