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3-Benzyl-1-butylimidazo[1,2-*a*]benzothieno[3,2-*d*]pyrimidine-2,5(1*H*,3*H*)-dione

Min-Hui Cao,[a] Jun Zhu[b] and De-Jiang Ni[c]*

[a]College of Science, HuaZhong Agricultural University, Wuhan 430070, People's Republic of China, [b]Department of Biochemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China, and [c]College of Horticulture and Forestry Science, HuaZhong Agricultural University, Wuhan 430070, People's Republic of China
Correspondence e-mail: nidejiang1021@yahoo.com.cn

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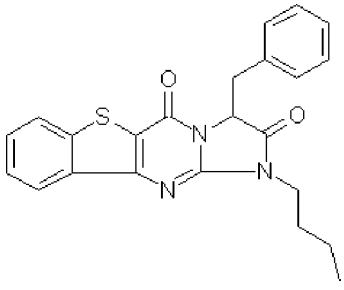
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.058; wR factor = 0.170; data-to-parameter ratio = 13.6.

In the crystal structure of the title compound, $C_{23}H_{21}N_3O_2S$, all ring atoms of the imidazo[1,2-*a*]benzothieno[3,2-*d*]-pyrimidine system are essentially coplanar and the phenyl ring is twisted with respect to it [dihedral angle = 72.60 (9)°]. The crystal packing is mainly governed by C—H$\cdots\pi$ hydrogen bonds and intermolecular π–π interactions, with interplanar distances of 3.54 (1) and 3.56 (1) Å, and with distances between adjacent ring centroids of 3.72 (1) and 3.80 (1) Å. The three terminal C atoms of the butyl group are disordered over two positions; the site occupancy factors are *ca* 0.6 and 0.4.

Related literature

Related preparation and biological activity is described by Walter (1999*a*,*b*). For related literature, see: Ding *et al.* (2004); Janiak (2000). For the crystal structures of other fused pyrimidinone derivatives, see: Cao *et al.* (2006); Xu *et al.* (2005).



Experimental

Crystal data

$C_{23}H_{21}N_3O_2S$
M_r = 403.49
Monoclinic, $P2_1/n$
a = 13.1732 (16) Å
b = 8.4957 (11) Å
c = 18.584 (2) Å
β = 103.345 (2)°
V = 2023.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.26 × 0.16 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.954, T_{max} = 0.982
15534 measured reflections
3958 independent reflections
2896 reflections with $I > 2\sigma(I)$
R_{int} = 0.129

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.170
S = 1.00
3958 reflections
292 parameters
22 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

*Cg*5 is the centroid of the C18–C23 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$\cdots$*Cg*5^{i}	0.96	2.81	3.682 (3)	156

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2501).

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supplementary materials

Acta Cryst. (2008). E**64**, o10 [**doi:10.1107/S1600536807061521**]

3-Benzyl-1-butylimidazo[1,2-*a*]benzothieno[3,2-*d*]pyrimidine-2,5(1*H*,3*H*)-dione

M.-H. Cao, J. Zhu and D.-J. Ni

Comment

In the field of bioactive molecules, thienopyrimidine have received a great deal of attention (Walter, 1999*a*,b). Recently, There have being focused on the synthesis of the fused heterocycle systems containing thienopyrimidine *via* aza-Wittig reaction at room temperature(Ding *et al.*, 2004). Herein, we present X-ray crystallographic analysis of the compound (I) in this paper, (Fig. 1), which may be used as a new precursor for obtaining bioactive molecules.

In the molecule, the bond lengths and angles are unexceptional (Cao *et al.*, 2006; Xu *et al.*, 2005). The four fused rings are close to coplanarity, with maximum deviations 0.060 (2)Å and −0.033 (3)Å for O3 and C11, respectively, which forms a dihedral angle of 72.60 (9)° with the adjacent C18—C23 phenyl ring.

Intermolecular C—H···π hydrogen bonds (Table 2) seem to be effective in stabilizing the crystal structure. Further stability the crystal structure is provided by offset π-π stacking interactions (Janiak, 2000) involving the thiophene (A), the imidazoe (B) and the C1—C6 benzene (C) rings. The A:*C* interplanar distance is 3.54 (1) Å with distances between adjacent ring centroids of 3.72 (1)Å (symmetry code relating the adjacent rings: 1 − *x*, 2 − *y*, −*z*). A further interaction occurs between B adjacent C rings (symmetry code: 1 − *x*, 1 − *y*, −*z*), with an interplanar distance of 3.56 (1)Å and a centroid-to-centroid distance of 3.80 (1)Å (Fig. 2).

Experimental

To a solution of the ethyl 3-((butylimino)methyleneamino)benzothiophene-2-carboxylate (3 mmol) in dichloromethane (5 ml) was added ethyl 2-amino-3-phenylpropanoate (3 mmol). After stirring the reaction mixture for 2 h, the solvent was removed and anhydrous ethanol (10 ml) with several drops of EtONa in EtOH was added. The mixture was stirred for 5 h at room temperature. The solution was concentrated under reduced pressure and the residue was recrystallized from ethanol to give the title compound in a yield of 86%. Crystals suitable for single-crystal X-ray diffraction were obtained by recrystallization from a mixed solvent of ethanol and dichloromethane (1:3 *v*/*v*) at room temperature.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for Csp^2, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, C—H = 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3. C14, C15, C16 and attached hydrogen atoms are disordered over two sites, with refined occupancies of 0.387 (9) and 0.613 (9).

Figures

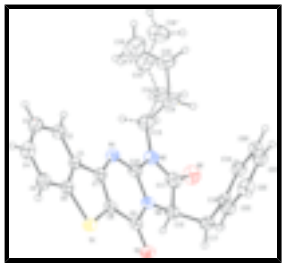


Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Only the major disorder component is shown.

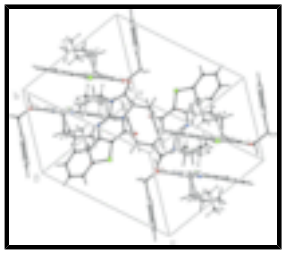


Fig. 2. The packing of the title compound.

3-Benzyl-1-butylimidazo[1,2-*a*]benzothieno[3,2-*d*]pyrimidine- 2,5(1*H*,3*H*)-dione

Crystal data

$C_{23}H_{21}N_3O_2S$	F_{000} = 848
M_r = 403.49	D_x = 1.324 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3589 reflections
a = 13.1732 (16) Å	θ = 2.3–23.5º
b = 8.4957 (11) Å	μ = 0.18 mm^{-1}
c = 18.584 (2) Å	T = 298 (2) K
β = 103.345 (2)º	Prism, colourless
V = 2023.7 (4) Å^3	0.26 × 0.16 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area0detector diffractometer	3958 independent reflections
Radiation source: fine-focus sealed tube	2896 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.129
T = 298(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −16→16
T_{min} = 0.954, T_{max} = 0.982	k = −10→10
15534 measured reflections	l = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.059$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
3958 reflections	$\Delta\rho_{max} = 0.26$ e Å^{-3}
292 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
22 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)
C1	0.45304 (17)	0.7981 (3)	0.00701 (13)	0.0455 (6)	
C2	0.40479 (19)	0.8227 (3)	−0.06750 (13)	0.0541 (6)	
H2	0.4330	0.7798	−0.1046	0.065*	
C3	0.31509 (19)	0.9112 (3)	−0.08510 (14)	0.0613 (7)	
H3	0.2828	0.9287	−0.1345	0.074*	
C4	0.27219 (19)	0.9745 (3)	−0.03029 (15)	0.0658 (8)	
H4	0.2111	1.0332	−0.0435	0.079*	
C5	0.31784 (19)	0.9528 (3)	0.04333 (15)	0.0605 (7)	
H5	0.2883	0.9956	0.0798	0.073*	
C6	0.40899 (17)	0.8655 (3)	0.06174 (13)	0.0500 (6)	
C7	0.54724 (16)	0.7149 (3)	0.03847 (12)	0.0441 (5)	
C8	0.57103 (17)	0.7199 (3)	0.11501 (12)	0.0465 (6)	
C9	0.66293 (18)	0.6487 (3)	0.15852 (12)	0.0497 (6)	
C10	0.68847 (18)	0.5729 (3)	0.03767 (12)	0.0454 (5)	
C11	0.8372 (2)	0.4266 (3)	0.06606 (15)	0.0563 (6)	
C12	0.81459 (18)	0.4798 (3)	0.13877 (14)	0.0544 (6)	
H12	0.7970	0.3870	0.1648	0.065*	

C13	0.7543 (2)	0.4725 (3)	−0.06900 (13)	0.0638 (7)	
H13A	0.6849	0.4359	−0.0928	0.077*	0.613 (9)
H13B	0.8029	0.3908	−0.0754	0.077*	0.613 (9)
H13C	0.6838	0.4415	−0.0932	0.077*	0.387 (9)
H13D	0.8002	0.3872	−0.0756	0.077*	0.387 (9)
C14	0.8106 (7)	0.6116 (9)	−0.0933 (4)	0.062 (2)	0.613 (9)
H14A	0.8832	0.6084	−0.0668	0.074*	0.613 (9)
H14B	0.7807	0.7079	−0.0793	0.074*	0.613 (9)
C15	0.8060 (5)	0.6175 (9)	−0.1761 (3)	0.087 (2)	0.613 (9)
H15A	0.8560	0.6945	−0.1852	0.105*	0.613 (9)
H15B	0.8260	0.5156	−0.1920	0.105*	0.613 (9)
C16	0.7009 (7)	0.6589 (14)	−0.2207 (5)	0.154 (4)	0.613 (9)
H16A	0.6520	0.5788	−0.2150	0.230*	0.613 (9)
H16B	0.7031	0.6667	−0.2719	0.230*	0.613 (9)
H16C	0.6797	0.7580	−0.2042	0.230*	0.613 (9)
C14'	0.7768 (13)	0.6158 (15)	−0.1097 (5)	0.076 (4)	0.387 (9)
H14C	0.8496	0.6457	−0.0940	0.091*	0.387 (9)
H14D	0.7337	0.7037	−0.1018	0.091*	0.387 (9)
C15'	0.7494 (10)	0.5634 (13)	−0.1926 (4)	0.101 (4)	0.387 (9)
H15C	0.7920	0.4746	−0.2002	0.121*	0.387 (9)
H15D	0.6765	0.5343	−0.2083	0.121*	0.387 (9)
C16'	0.7727 (11)	0.7057 (14)	−0.2344 (5)	0.117 (4)	0.387 (9)
H16D	0.7340	0.7943	−0.2230	0.175*	0.387 (9)
H16E	0.7528	0.6849	−0.2866	0.175*	0.387 (9)
H16F	0.8460	0.7285	−0.2204	0.175*	0.387 (9)
C17	0.90741 (18)	0.5630 (3)	0.18900 (13)	0.0555 (7)	
H17A	0.8906	0.5818	0.2364	0.067*	
H17B	0.9667	0.4920	0.1975	0.067*	
C18	0.93996 (16)	0.7166 (3)	0.16112 (12)	0.0475 (6)	
C19	0.99200 (17)	0.7229 (3)	0.10411 (13)	0.0509 (6)	
H19	1.0040	0.6301	0.0808	0.061*	
C20	1.02611 (18)	0.8632 (3)	0.08140 (14)	0.0543 (6)	
H20	1.0604	0.8644	0.0429	0.065*	
C21	1.00975 (19)	1.0019 (3)	0.11538 (14)	0.0593 (7)	
H21	1.0336	1.0966	0.1004	0.071*	
C22	0.9581 (2)	0.9992 (3)	0.17149 (15)	0.0643 (7)	
H22	0.9465	1.0925	0.1945	0.077*	
C23	0.92311 (19)	0.8578 (3)	0.19387 (13)	0.0575 (7)	
H23	0.8876	0.8575	0.2317	0.069*	
N1	0.60676 (14)	0.6380 (2)	−0.00223 (10)	0.0468 (5)	
N2	0.75950 (15)	0.4872 (2)	0.01036 (11)	0.0521 (5)	
N3	0.72009 (13)	0.5741 (2)	0.11365 (9)	0.0476 (5)	
O1	0.69271 (13)	0.6488 (2)	0.22618 (9)	0.0653 (5)	
O2	0.91073 (15)	0.3495 (2)	0.05804 (11)	0.0710 (6)	
S1	0.48079 (5)	0.82378 (9)	0.15079 (3)	0.0585 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0434 (12)	0.0490 (14)	0.0430 (12)	−0.0121 (10)	0.0076 (10)	−0.0026 (10)
C2	0.0530 (14)	0.0616 (16)	0.0450 (13)	−0.0097 (12)	0.0054 (11)	−0.0037 (11)
C3	0.0555 (15)	0.0682 (18)	0.0539 (14)	−0.0071 (13)	−0.0001 (12)	0.0033 (13)
C4	0.0513 (15)	0.0627 (18)	0.0779 (19)	0.0005 (13)	0.0037 (14)	−0.0013 (15)
C5	0.0517 (14)	0.0638 (17)	0.0666 (16)	−0.0008 (12)	0.0149 (12)	−0.0094 (13)
C6	0.0454 (13)	0.0577 (15)	0.0463 (13)	−0.0114 (11)	0.0093 (11)	−0.0051 (11)
C7	0.0422 (12)	0.0504 (14)	0.0396 (11)	−0.0098 (10)	0.0092 (10)	−0.0035 (10)
C8	0.0448 (12)	0.0572 (15)	0.0391 (12)	−0.0085 (11)	0.0132 (10)	−0.0015 (10)
C9	0.0477 (13)	0.0636 (16)	0.0390 (12)	−0.0122 (11)	0.0124 (10)	0.0058 (11)
C10	0.0520 (13)	0.0441 (13)	0.0422 (12)	−0.0078 (11)	0.0150 (11)	−0.0013 (10)
C11	0.0602 (15)	0.0419 (14)	0.0678 (16)	−0.0027 (12)	0.0170 (13)	0.0062 (12)
C12	0.0559 (14)	0.0524 (15)	0.0562 (14)	−0.0005 (11)	0.0154 (12)	0.0185 (12)
C13	0.0673 (16)	0.0719 (19)	0.0535 (15)	0.0011 (14)	0.0163 (13)	−0.0162 (14)
C14	0.079 (5)	0.065 (4)	0.041 (3)	0.019 (3)	0.013 (3)	0.008 (3)
C15	0.101 (5)	0.110 (5)	0.047 (3)	−0.012 (4)	0.010 (3)	0.005 (3)
C16	0.141 (7)	0.175 (8)	0.118 (6)	−0.013 (6)	−0.023 (5)	0.032 (5)
C14'	0.096 (11)	0.095 (8)	0.037 (5)	0.030 (6)	0.014 (6)	0.017 (5)
C15'	0.074 (8)	0.147 (12)	0.077 (7)	−0.010 (7)	0.005 (6)	−0.006 (7)
C16'	0.137 (8)	0.130 (8)	0.089 (6)	−0.019 (6)	0.037 (6)	0.030 (6)
C17	0.0504 (13)	0.0694 (18)	0.0454 (13)	0.0088 (12)	0.0080 (11)	0.0162 (12)
C18	0.0373 (11)	0.0619 (16)	0.0397 (12)	0.0052 (11)	0.0017 (10)	0.0068 (11)
C19	0.0527 (13)	0.0534 (15)	0.0484 (13)	0.0044 (11)	0.0151 (11)	−0.0039 (11)
C20	0.0549 (14)	0.0576 (17)	0.0543 (14)	0.0015 (12)	0.0208 (12)	0.0027 (12)
C21	0.0570 (14)	0.0509 (15)	0.0690 (17)	−0.0023 (12)	0.0125 (13)	0.0031 (13)
C22	0.0655 (16)	0.0589 (18)	0.0679 (17)	0.0055 (14)	0.0138 (14)	−0.0143 (14)
C23	0.0510 (14)	0.077 (2)	0.0451 (13)	0.0078 (13)	0.0125 (11)	−0.0049 (13)
N1	0.0472 (11)	0.0540 (12)	0.0394 (10)	−0.0041 (9)	0.0104 (9)	−0.0025 (9)
N2	0.0554 (11)	0.0516 (12)	0.0513 (11)	0.0024 (9)	0.0163 (10)	−0.0016 (9)
N3	0.0447 (10)	0.0579 (13)	0.0406 (10)	−0.0026 (9)	0.0106 (9)	0.0074 (9)
O1	0.0580 (10)	0.1020 (15)	0.0363 (9)	−0.0023 (10)	0.0116 (8)	0.0123 (9)
O2	0.0705 (12)	0.0522 (11)	0.0911 (14)	0.0144 (9)	0.0202 (11)	−0.0008 (10)
S1	0.0510 (4)	0.0854 (6)	0.0405 (4)	−0.0052 (3)	0.0131 (3)	−0.0096 (3)

Geometric parameters (Å, °)

C1—C2	1.400 (3)	C13—H13D	0.9700
C1—C6	1.404 (3)	C14—C15	1.527 (7)
C1—C7	1.431 (3)	C14—H14A	0.9700
C2—C3	1.375 (4)	C14—H14B	0.9700
C2—H2	0.9300	C15—C16	1.482 (8)
C3—C4	1.383 (4)	C15—H15A	0.9700
C3—H3	0.9300	C15—H15B	0.9700
C4—C5	1.374 (3)	C16—H16A	0.9600
C4—H4	0.9300	C16—H16B	0.9600
C5—C6	1.385 (3)	C16—H16C	0.9600

C5—H5	0.9300	C14'—C15'	1.564 (9)
C6—S1	1.743 (2)	C14'—H14C	0.9700
C7—N1	1.373 (3)	C14'—H14D	0.9700
C7—C8	1.385 (3)	C15'—C16'	1.506 (9)
C8—C9	1.426 (3)	C15'—H15C	0.9700
C8—S1	1.732 (2)	C15'—H15D	0.9700
C9—O1	1.228 (3)	C16'—H16D	0.9600
C9—N3	1.398 (3)	C16'—H16E	0.9600
C10—N1	1.283 (3)	C16'—H16F	0.9600
C10—N2	1.372 (3)	C17—C18	1.503 (3)
C10—N3	1.377 (3)	C17—H17A	0.9700
C11—O2	1.207 (3)	C17—H17B	0.9700
C11—N2	1.377 (3)	C18—C23	1.386 (3)
C11—C12	1.518 (4)	C18—C19	1.389 (3)
C12—N3	1.463 (3)	C19—C20	1.374 (3)
C12—C17	1.529 (3)	C19—H19	0.9300
C12—H12	0.9800	C20—C21	1.377 (3)
C13—N2	1.466 (3)	C20—H20	0.9300
C13—C14'	1.498 (9)	C21—C22	1.371 (4)
C13—C14	1.519 (7)	C21—H21	0.9300
C13—H13A	0.9700	C22—C23	1.385 (4)
C13—H13B	0.9700	C22—H22	0.9300
C13—H13C	0.9700	C23—H23	0.9300
C2—C1—C6	119.1 (2)	C13—C14—H14A	108.6
C2—C1—C7	129.1 (2)	C15—C14—H14A	108.6
C6—C1—C7	111.7 (2)	C13—C14—H14B	108.6
C3—C2—C1	119.1 (2)	C15—C14—H14B	108.6
C3—C2—H2	120.5	H14A—C14—H14B	107.6
C1—C2—H2	120.5	C16—C15—C14	112.8 (6)
C2—C3—C4	120.8 (2)	C16—C15—H15A	109.0
C2—C3—H3	119.6	C14—C15—H15A	109.0
C4—C3—H3	119.6	C16—C15—H15B	109.0
C5—C4—C3	121.5 (2)	C14—C15—H15B	109.0
C5—C4—H4	119.3	H15A—C15—H15B	107.8
C3—C4—H4	119.3	C15—C16—H16A	109.5
C4—C5—C6	118.2 (2)	C15—C16—H16B	109.5
C4—C5—H5	120.9	H16A—C16—H16B	109.5
C6—C5—H5	120.9	C15—C16—H16C	109.5
C5—C6—C1	121.3 (2)	H16A—C16—H16C	109.5
C5—C6—S1	126.4 (2)	H16B—C16—H16C	109.5
C1—C6—S1	112.37 (18)	C13—C14'—C15'	103.8 (7)
N1—C7—C8	123.9 (2)	C13—C14'—H14C	111.0
N1—C7—C1	124.2 (2)	C15'—C14'—H14C	111.0
C8—C7—C1	111.9 (2)	C13—C14'—H14D	111.0
C7—C8—C9	122.0 (2)	C15'—C14'—H14D	111.0
C7—C8—S1	113.44 (18)	H14C—C14'—H14D	109.0
C9—C8—S1	124.51 (17)	C16'—C15'—C14'	104.6 (7)
O1—C9—N3	121.5 (2)	C16'—C15'—H15C	110.8
O1—C9—C8	127.5 (2)	C14'—C15'—H15C	110.8

N3—C9—C8	110.96 (19)	C16'—C15'—H15D	110.8
N1—C10—N2	124.6 (2)	C14'—C15'—H15D	110.8
N1—C10—N3	127.2 (2)	H15C—C15'—H15D	108.9
N2—C10—N3	108.2 (2)	C18—C17—C12	116.25 (18)
O2—C11—N2	126.1 (3)	C18—C17—H17A	108.2
O2—C11—C12	126.8 (2)	C12—C17—H17A	108.2
N2—C11—C12	107.1 (2)	C18—C17—H17B	108.2
N3—C12—C11	101.91 (19)	C12—C17—H17B	108.2
N3—C12—C17	116.3 (2)	H17A—C17—H17B	107.4
C11—C12—C17	112.8 (2)	C23—C18—C19	117.3 (2)
N3—C12—H12	108.5	C23—C18—C17	120.9 (2)
C11—C12—H12	108.5	C19—C18—C17	121.8 (2)
C17—C12—H12	108.5	C20—C19—C18	121.4 (2)
N2—C13—C14'	118.0 (5)	C20—C19—H19	119.3
N2—C13—C14	108.7 (3)	C18—C19—H19	119.3
C14'—C13—C14	18.3 (7)	C19—C20—C21	120.3 (2)
N2—C13—H13A	107.8	C19—C20—H20	119.9
C14'—C13—H13A	107.8	C21—C20—H20	119.9
C14—C13—H13A	126.0	C22—C21—C20	119.5 (3)
N2—C13—H13B	107.8	C22—C21—H21	120.2
C14'—C13—H13B	107.8	C20—C21—H21	120.2
C14—C13—H13B	97.9	C21—C22—C23	120.0 (2)
H13A—C13—H13B	107.1	C21—C22—H22	120.0
N2—C13—H13C	107.9	C23—C22—H22	120.0
C14'—C13—H13C	105.5	C18—C23—C22	121.4 (2)
C14—C13—H13C	123.7	C18—C23—H23	119.3
H13A—C13—H13C	2.9	C22—C23—H23	119.3
H13B—C13—H13C	109.7	C10—N1—C7	113.33 (18)
N2—C13—H13D	107.8	C10—N2—C11	111.9 (2)
C14'—C13—H13D	109.9	C10—N2—C13	122.7 (2)
C14—C13—H13D	100.5	C11—N2—C13	125.4 (2)
H13A—C13—H13D	104.6	C10—N3—C9	122.56 (19)
H13B—C13—H13D	2.8	C10—N3—C12	110.89 (19)
H13C—C13—H13D	107.2	C9—N3—C12	126.42 (18)
C13—C14—C15	114.6 (6)	C8—S1—C6	90.52 (11)
C6—C1—C2—C3	−0.5 (3)	C18—C19—C20—C21	0.4 (4)
C7—C1—C2—C3	−178.2 (2)	C19—C20—C21—C22	−0.8 (4)
C1—C2—C3—C4	−0.4 (4)	C20—C21—C22—C23	0.3 (4)
C2—C3—C4—C5	0.6 (4)	C19—C18—C23—C22	−1.0 (3)
C3—C4—C5—C6	0.2 (4)	C17—C18—C23—C22	176.2 (2)
C4—C5—C6—C1	−1.2 (4)	C21—C22—C23—C18	0.6 (4)
C4—C5—C6—S1	179.5 (2)	N2—C10—N1—C7	178.9 (2)
C2—C1—C6—C5	1.3 (3)	N3—C10—N1—C7	−0.4 (3)
C7—C1—C6—C5	179.4 (2)	C8—C7—N1—C10	−1.2 (3)
C2—C1—C6—S1	−179.29 (18)	C1—C7—N1—C10	179.3 (2)
C7—C1—C6—S1	−1.2 (2)	N1—C10—N2—C11	−177.8 (2)
C2—C1—C7—N1	−2.0 (4)	N3—C10—N2—C11	1.6 (3)
C6—C1—C7—N1	−179.8 (2)	N1—C10—N2—C13	5.6 (4)
C2—C1—C7—C8	178.4 (2)	N3—C10—N2—C13	−174.9 (2)

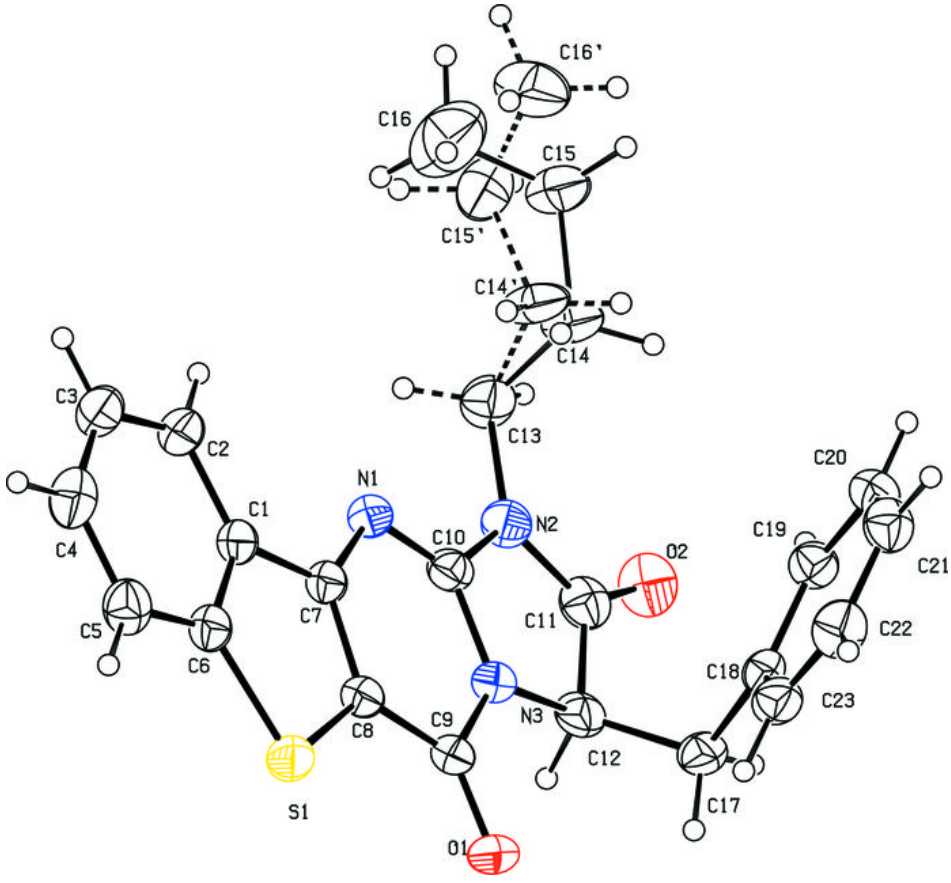
C6—C1—C7—C8	0.6 (3)	O2—C11—N2—C10	−178.5 (2)
N1—C7—C8—C9	2.1 (4)	C12—C11—N2—C10	−0.3 (3)
C1—C7—C8—C9	−178.3 (2)	O2—C11—N2—C13	−2.0 (4)
N1—C7—C8—S1	−179.33 (17)	C12—C11—N2—C13	176.1 (2)
C1—C7—C8—S1	0.3 (3)	C14'—C13—N2—C10	69.0 (8)
C7—C8—C9—O1	178.4 (2)	C14—C13—N2—C10	86.1 (5)
S1—C8—C9—O1	0.0 (4)	C14'—C13—N2—C11	−107.1 (8)
C7—C8—C9—N3	−1.4 (3)	C14—C13—N2—C11	−90.0 (5)
S1—C8—C9—N3	−179.76 (16)	N1—C10—N3—C9	1.0 (4)
O2—C11—C12—N3	177.1 (2)	N2—C10—N3—C9	−178.42 (19)
N2—C11—C12—N3	−1.0 (2)	N1—C10—N3—C12	177.1 (2)
O2—C11—C12—C17	51.7 (3)	N2—C10—N3—C12	−2.3 (2)
N2—C11—C12—C17	−126.5 (2)	O1—C9—N3—C10	−179.8 (2)
N2—C13—C14—C15	−176.5 (5)	C8—C9—N3—C10	0.0 (3)
C14'—C13—C14—C15	−53 (2)	O1—C9—N3—C12	4.7 (4)
C13—C14—C15—C16	71.4 (10)	C8—C9—N3—C12	−175.5 (2)
N2—C13—C14'—C15'	−172.5 (7)	C11—C12—N3—C10	2.0 (2)
C14—C13—C14'—C15'	124 (3)	C17—C12—N3—C10	125.1 (2)
C13—C14'—C15'—C16'	−179.4 (12)	C11—C12—N3—C9	177.9 (2)
N3—C12—C17—C18	−52.3 (3)	C17—C12—N3—C9	−59.0 (3)
C11—C12—C17—C18	65.0 (3)	C7—C8—S1—C6	−0.82 (19)
C12—C17—C18—C23	109.3 (3)	C9—C8—S1—C6	177.7 (2)
C12—C17—C18—C19	−73.6 (3)	C5—C6—S1—C8	−179.5 (2)
C23—C18—C19—C20	0.5 (3)	C1—C6—S1—C8	1.17 (18)
C17—C18—C19—C20	−176.7 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Cg5^{i}	0.96	2.81	3.682 (3)	156

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

Fig. 1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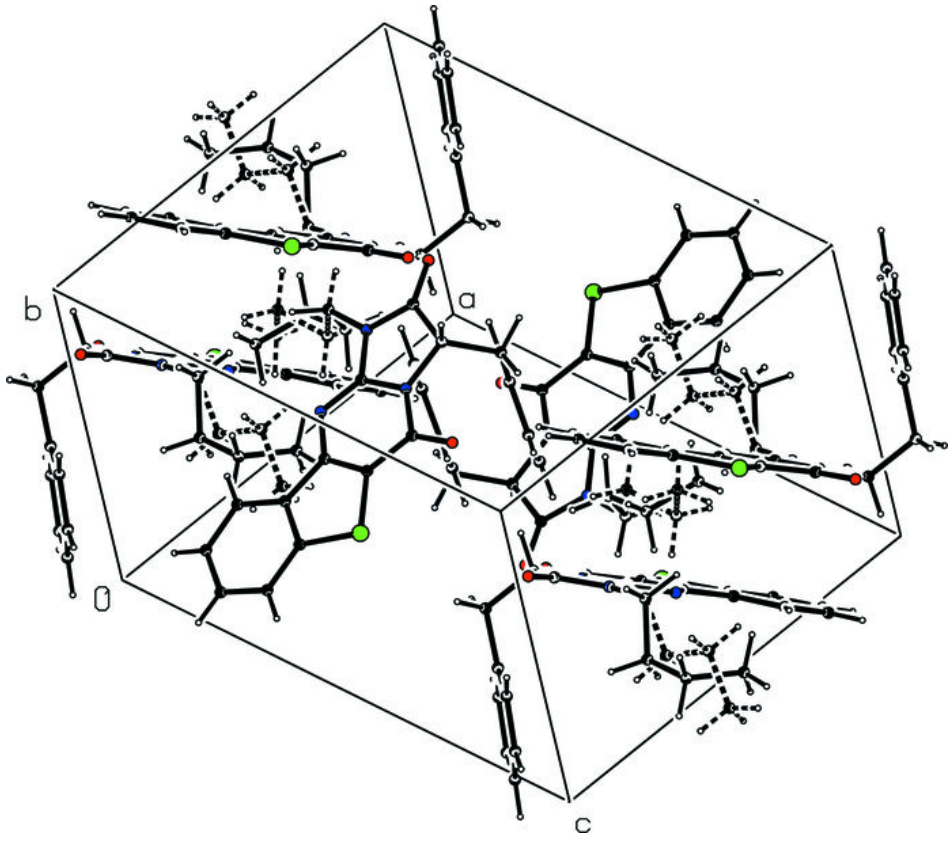
Fig. 2