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2-Butylamino-3-(4-fluorophenyl)-6,8-diphenyl-3,5,6,8-tetrahydro-4*H*-thiopyrano[4′,3′:4,5]thieno[2,3-*d*]pyrimidin-4-one

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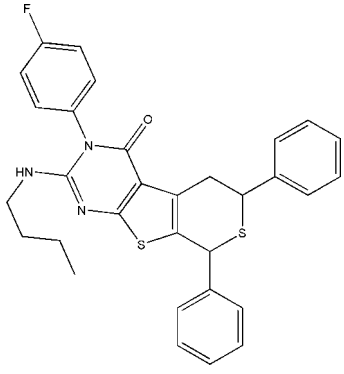
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.063; wR factor = 0.218; data-to-parameter ratio = 13.6.

In the title molecule, $C_{31}H_{28}FN_3OS_2$, the two fused rings of the thieno[3,2-*d*]pyrimidine group form a dihedral angle of 4.99 (12)°, and the benzene ring of the 4-fluorophenyl group forms a dihedral angle of 77.44 (15)° with the pyrimidine ring. The thiopyran ring is in a half-chair conformation. The crystal packing is stabilized by weak intermolecular C—H···N hydrogen bonds and weak π–π interactions with a centroid–centroid distance of 3.900 (1) Å. The C atoms of the *n*-butyl group are disordered over two sites with approximate occupancies of 0.60 and 0.40.

Related literature

The preparation and biological activity is described by Walter (1999*a*,*b*). For related literature, see: Ding *et al.* (2004); Allen *et al.* (1987); Janiak (2000).



Experimental

Crystal data

$C_{31}H_{28}FN_3OS_2$
M_r = 541.68
Monoclinic, $P2_1/c$
a = 12.9430 (10) Å
b = 19.2323 (15) Å
c = 11.9433 (19) Å
β = 107.916 (2)°
V = 2828.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 294 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.957, T_{max} = 0.978
22538 measured reflections
4926 independent reflections
3496 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.218
S = 1.04
4926 reflections
361 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···N2^{i}	0.98	2.60	3.507 (4)	154

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

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: LH2571).

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supplementary materials

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2-Butylamino-3-(4-fluorophenyl)-6,8-diphenyl-3,5,6,8-tetrahydro-4*H*-thiopyrano[4',3':4,5]thieno[2,3-*d*]pyrimidin-4-one

W.-J. Li, R. Li, W.-Q. Wang and Y. Zhong

Comment

Thienopyrimidine derivatives are great inoprtance because of their remarkable biological properties, including antibacterial, antiallergic and antiinflammatory (Walter, 1999*a*,b). In recent years, we have been engaged in the prepation of heterocyclic derivatives containiing a fused pyrimidinone system using an aza-Wittig reaction (Ding *et al.*, 2004). We present here the structure of one such thiopyranothieno[2,3-*d*]pyrimidine derivative, (I) (Fig. 1), which has potential for use as a precursor for obtaining bioactive molecules. The bond lengths and angles are unexceptional (Allen *et al.*, 1987). The thieno (A), the pyrimidinone (B) and the C6—C11 phenyl (C), the C12—C17 phenyl (D), the C22—C27 benzene (E), rings are essentially planar and the dihedral angles between them are A/B = 4.99 (12)°, A/C = 67.4 (2)°, A/D = 82.2 (2)°, B/E = 77.44 (15)°. The thiopyrano ring is in a half-chair conformation [φ =213.6 (3)° and θ =130.6 (3)°, Puckering Amplitude =0.622 (2) Å]. Atoms C29, C30, C31 and attached hydrogen atoms are disordered over two sites, with refined occupancies of 0.396 (7) and 0.604 (7). Intermolecular C—H···N hydrogen bonds appear to be effective in stabilizing the crystal structure (Fig. 2, Table 1). Further stability is provided by offset π-π stacking interactions (Janiak, 2000) of symmetry related S2/C3/C4/C18/C19 rings (symmetry code: $1-x, -y, 1-z$), with an interplanar distance of 3.578 (1)Å and a centroid-to-centroid distance of 3.900 (1).

Refinement

All H atoms were located in difference maps and treated as riding atoms, with N—H = 0.86 Å, $U_{iso} = 1.2U_{eq}$ (N) for NH, C—H = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for Csp^2, C—H = 0.98 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH, 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.

Figures

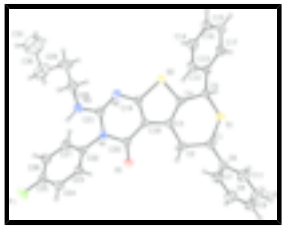

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Only the major disorder component is shown.

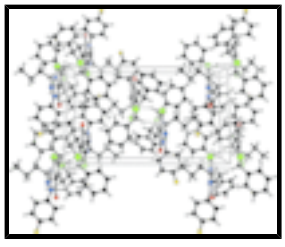

Fig. 2. The packing in the crystal structure, showing the C—H···N hydrogen bonds as dashed lines.

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Crystal data

$C_{31}H_{28}FN_3OS_2$	F_{000} = 1136
M_r = 541.68	D_x = 1.272 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7165 reflections
a = 12.9430 (10) Å	θ = 2.3–26.6º
b = 19.2323 (15) Å	μ = 0.22 mm^{-1}
c = 11.9433 (19) Å	T = 294 (2) K
β = 107.916 (2)º	Block, colorless
V = 2828.8 (5) Å^3	0.20 × 0.10 × 0.10 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	4926 independent reflections
Radiation source: fine-focus sealed tube	3496 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.039
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −15→15
T_{min} = 0.957, T_{max} = 0.978	k = −22→22
22538 measured reflections	l = −14→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.063	H-atom parameters constrained
$wR(F^2)$ = 0.218	$w = 1/[\sigma^2(F_o^2) + (0.1581P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max} < 0.001$
4926 reflections	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
361 parameters	$\Delta\rho_{min}$ = −0.33 e Å^{-3}
6 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	0.8214 (2)	0.48052 (16)	0.6797 (2)	0.0546 (7)	
H1	0.7860	0.5241	0.6460	0.066*	
C2	0.7483 (2)	0.44333 (16)	0.7389 (2)	0.0540 (7)	
H2A	0.7838	0.4010	0.7756	0.065*	
H2B	0.7377	0.4729	0.8003	0.065*	
C3	0.6392 (2)	0.42529 (13)	0.6531 (2)	0.0445 (6)	
C4	0.6206 (2)	0.41847 (13)	0.5352 (2)	0.0467 (6)	
C5	0.6986 (2)	0.42672 (14)	0.4652 (2)	0.0499 (7)	
H5	0.6839	0.4714	0.4239	0.060*	
C6	0.9332 (3)	0.49748 (18)	0.7595 (3)	0.0620 (8)	
C7	0.9944 (3)	0.4521 (3)	0.8420 (3)	0.0891 (12)	
H7	0.9663	0.4086	0.8507	0.107*	
C8	1.0967 (4)	0.4700 (3)	0.9120 (4)	0.1054 (15)	
H8	1.1363	0.4382	0.9675	0.126*	
C9	1.1408 (4)	0.5315 (3)	0.9027 (4)	0.1058 (16)	
H9	1.2107	0.5424	0.9497	0.127*	
C10	1.0824 (5)	0.5770 (4)	0.8244 (6)	0.151 (3)	
H10	1.1117	0.6203	0.8173	0.181*	
C11	0.9783 (4)	0.5607 (3)	0.7533 (5)	0.1189 (19)	
H11	0.9387	0.5937	0.7005	0.143*	
C12	0.6877 (2)	0.36995 (15)	0.3746 (2)	0.0498 (7)	
C13	0.6964 (3)	0.30109 (16)	0.4072 (3)	0.0716 (10)	
H13	0.7111	0.2893	0.4861	0.086*	
C14	0.6836 (4)	0.2490 (2)	0.3238 (3)	0.0862 (12)	
H14	0.6888	0.2026	0.3466	0.103*	
C15	0.6632 (4)	0.2661 (2)	0.2081 (3)	0.0889 (13)	
H15	0.6549	0.2312	0.1521	0.107*	
C16	0.6550 (3)	0.3340 (2)	0.1742 (3)	0.0833 (12)	
H16	0.6412	0.3453	0.0953	0.100*	
C17	0.6673 (3)	0.38626 (18)	0.2573 (3)	0.0640 (8)	
H17	0.6616	0.4326	0.2338	0.077*	
C18	0.5413 (2)	0.41524 (13)	0.6844 (2)	0.0419 (6)	
C19	0.4515 (2)	0.40394 (13)	0.5888 (2)	0.0456 (6)	

C20	0.5285 (2)	0.41069 (13)	0.7992 (2)	0.0443 (6)	
C21	0.3346 (2)	0.39246 (15)	0.6934 (2)	0.0497 (7)	
C22	0.4028 (2)	0.37698 (14)	0.9065 (2)	0.0473 (6)	
C23	0.3956 (2)	0.42682 (15)	0.9860 (2)	0.0528 (7)	
H23	0.4021	0.4736	0.9697	0.063*	
C24	0.3788 (3)	0.40724 (17)	1.0902 (3)	0.0625 (8)	
H24	0.3762	0.4402	1.1462	0.075*	
C25	0.3661 (3)	0.33909 (18)	1.1087 (3)	0.0667 (9)	
C26	0.3731 (3)	0.28827 (18)	1.0313 (3)	0.0728 (10)	
H26	0.3643	0.2417	1.0472	0.087*	
C27	0.3936 (3)	0.30789 (15)	0.9292 (3)	0.0617 (8)	
H27	0.4011	0.2744	0.8760	0.074*	
C28	0.1356 (3)	0.3866 (3)	0.6054 (4)	0.1014 (15)	
H28A	0.1406	0.4237	0.5523	0.122*	0.604 (7)
H28B	0.0760	0.3982	0.6353	0.122*	0.604 (7)
H28C	0.1492	0.4031	0.5345	0.122*	0.396 (7)
H28D	0.0800	0.4154	0.6209	0.122*	0.396 (7)
C29	0.1060 (9)	0.3233 (6)	0.5360 (7)	0.132 (3)	0.604 (7)
H29A	0.1650	0.3077	0.5081	0.159*	0.604 (7)
H29B	0.0420	0.3306	0.4688	0.159*	0.604 (7)
C30	0.0837 (12)	0.2715 (7)	0.6196 (11)	0.168 (4)	0.604 (7)
H30A	0.0338	0.2897	0.6586	0.202*	0.604 (7)
H30B	0.1498	0.2561	0.6780	0.202*	0.604 (7)
C31	0.0308 (18)	0.2126 (10)	0.5299 (17)	0.270 (10)	0.604 (7)
H31A	0.0860	0.1896	0.5053	0.405*	0.604 (7)
H31B	−0.0220	0.2326	0.4626	0.405*	0.604 (7)
H31C	−0.0041	0.1796	0.5666	0.405*	0.604 (7)
C29'	0.0978 (16)	0.3103 (7)	0.5937 (13)	0.132 (3)	0.396 (7)
H29C	0.1595	0.2819	0.5928	0.159*	0.396 (7)
H29D	0.0802	0.2984	0.6647	0.159*	0.396 (7)
C30'	0.0013 (13)	0.2882 (10)	0.4884 (16)	0.168 (4)	0.396 (7)
H30C	−0.0566	0.2739	0.5190	0.202*	0.396 (7)
H30D	−0.0241	0.3293	0.4408	0.202*	0.396 (7)
C31'	0.016 (2)	0.2310 (14)	0.406 (2)	0.231 (13)	0.396 (7)
H31D	−0.0515	0.2241	0.3447	0.346*	0.396 (7)
H31E	0.0364	0.1887	0.4500	0.346*	0.396 (7)
H31F	0.0711	0.2443	0.3726	0.346*	0.396 (7)
F1	0.3479 (2)	0.31934 (13)	1.21011 (16)	0.0997 (8)	
N1	0.41996 (19)	0.39625 (11)	0.79666 (19)	0.0470 (6)	
N2	0.34648 (19)	0.39482 (12)	0.58824 (19)	0.0496 (6)	
N3	0.2334 (2)	0.38759 (16)	0.7029 (2)	0.0711 (8)	
H3	0.2273	0.3849	0.7725	0.085*	
O1	0.59961 (17)	0.41631 (10)	0.89348 (17)	0.0550 (5)	
S1	0.83816 (7)	0.42719 (5)	0.56027 (7)	0.0673 (3)	
S2	0.48421 (6)	0.40244 (4)	0.45975 (6)	0.0530 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0575 (18)	0.0556 (18)	0.0530 (16)	−0.0068 (14)	0.0203 (13)	−0.0060 (12)
C2	0.0538 (17)	0.0595 (18)	0.0506 (15)	−0.0040 (14)	0.0190 (13)	−0.0061 (13)
C3	0.0528 (16)	0.0364 (14)	0.0466 (14)	0.0020 (11)	0.0188 (12)	−0.0001 (10)
C4	0.0539 (17)	0.0405 (14)	0.0480 (14)	0.0007 (12)	0.0192 (12)	−0.0021 (11)
C5	0.0592 (18)	0.0456 (16)	0.0488 (14)	−0.0017 (13)	0.0221 (13)	−0.0006 (11)
C6	0.0585 (19)	0.074 (2)	0.0582 (17)	−0.0113 (16)	0.0242 (14)	−0.0108 (15)
C7	0.058 (2)	0.111 (3)	0.090 (3)	−0.009 (2)	0.0102 (19)	0.014 (2)
C8	0.067 (3)	0.148 (5)	0.091 (3)	−0.006 (3)	0.009 (2)	0.010 (3)
C9	0.068 (3)	0.158 (5)	0.086 (3)	−0.024 (3)	0.015 (2)	−0.033 (3)
C10	0.089 (4)	0.144 (5)	0.182 (6)	−0.054 (4)	−0.014 (4)	0.007 (4)
C11	0.095 (3)	0.111 (4)	0.120 (4)	−0.040 (3)	−0.011 (3)	0.021 (3)
C12	0.0574 (17)	0.0532 (17)	0.0459 (14)	−0.0032 (13)	0.0262 (13)	−0.0028 (12)
C13	0.117 (3)	0.0527 (19)	0.0595 (18)	−0.0032 (18)	0.0478 (19)	−0.0003 (14)
C14	0.134 (4)	0.056 (2)	0.087 (2)	−0.013 (2)	0.061 (3)	−0.0166 (18)
C15	0.119 (3)	0.083 (3)	0.082 (2)	−0.027 (2)	0.055 (2)	−0.036 (2)
C16	0.104 (3)	0.105 (3)	0.0460 (17)	−0.017 (2)	0.0309 (18)	−0.0122 (18)
C17	0.077 (2)	0.068 (2)	0.0514 (17)	−0.0019 (16)	0.0264 (16)	0.0066 (14)
C18	0.0420 (14)	0.0391 (14)	0.0463 (14)	0.0000 (11)	0.0162 (11)	−0.0006 (10)
C19	0.0510 (17)	0.0405 (14)	0.0465 (14)	0.0014 (12)	0.0166 (12)	0.0025 (10)
C20	0.0515 (16)	0.0370 (13)	0.0466 (14)	−0.0008 (11)	0.0182 (12)	−0.0035 (10)
C21	0.0478 (16)	0.0500 (17)	0.0530 (16)	0.0010 (12)	0.0179 (13)	0.0009 (12)
C22	0.0507 (16)	0.0470 (15)	0.0463 (14)	−0.0022 (12)	0.0179 (12)	−0.0016 (11)
C23	0.0610 (19)	0.0443 (16)	0.0569 (16)	0.0002 (13)	0.0237 (14)	−0.0050 (12)
C24	0.071 (2)	0.066 (2)	0.0547 (17)	−0.0014 (16)	0.0256 (16)	−0.0119 (14)
C25	0.082 (2)	0.073 (2)	0.0495 (16)	−0.0124 (17)	0.0271 (16)	0.0051 (15)
C26	0.100 (3)	0.0525 (19)	0.072 (2)	−0.0107 (17)	0.0353 (19)	0.0079 (15)
C27	0.086 (2)	0.0457 (16)	0.0592 (17)	−0.0053 (15)	0.0305 (16)	−0.0047 (13)
C28	0.050 (2)	0.174 (5)	0.078 (3)	−0.006 (3)	0.0180 (19)	0.017 (3)
C29	0.101 (5)	0.208 (10)	0.073 (6)	−0.018 (6)	0.005 (6)	−0.045 (7)
C30	0.148 (9)	0.126 (8)	0.206 (11)	−0.035 (7)	0.017 (7)	−0.010 (8)
C31	0.27 (2)	0.25 (2)	0.28 (2)	−0.034 (19)	0.07 (2)	−0.012 (19)
C29'	0.101 (5)	0.208 (10)	0.073 (6)	−0.018 (6)	0.005 (6)	−0.045 (7)
C30'	0.148 (9)	0.126 (8)	0.206 (11)	−0.035 (7)	0.017 (7)	−0.010 (8)
C31'	0.24 (3)	0.22 (3)	0.23 (3)	0.00 (2)	0.07 (3)	−0.03 (2)
F1	0.133 (2)	0.1177 (18)	0.0588 (11)	−0.0237 (15)	0.0443 (13)	0.0108 (11)
N1	0.0489 (14)	0.0494 (13)	0.0464 (12)	−0.0013 (10)	0.0201 (10)	−0.0026 (9)
N2	0.0431 (13)	0.0554 (14)	0.0492 (13)	−0.0015 (10)	0.0125 (10)	−0.0003 (10)
N3	0.0491 (16)	0.109 (2)	0.0588 (15)	−0.0030 (14)	0.0213 (12)	0.0037 (14)
O1	0.0544 (12)	0.0664 (13)	0.0432 (10)	−0.0070 (10)	0.0136 (9)	−0.0076 (9)
S1	0.0562 (5)	0.0893 (7)	0.0620 (5)	−0.0049 (4)	0.0264 (4)	−0.0186 (4)
S2	0.0561 (5)	0.0612 (5)	0.0416 (4)	−0.0025 (3)	0.0150 (3)	−0.0022 (3)

Geometric parameters (Å, °)

C1—C6	1.503 (4)	C21—N2	1.313 (4)

C1—C2	1.523 (4)	C21—N3	1.352 (4)
C1—S1	1.823 (3)	C21—N1	1.381 (4)
C1—H1	0.9800	C22—C27	1.369 (4)
C2—C3	1.508 (4)	C22—C23	1.372 (4)
C2—H2A	0.9700	C22—N1	1.444 (3)
C2—H2B	0.9700	C23—C24	1.381 (4)
C3—C4	1.360 (4)	C23—H23	0.9300
C3—C18	1.440 (4)	C24—C25	1.347 (5)
C4—C5	1.504 (4)	C24—H24	0.9300
C4—S2	1.745 (3)	C25—F1	1.357 (3)
C5—C12	1.513 (4)	C25—C26	1.367 (5)
C5—S1	1.814 (3)	C26—C27	1.378 (4)
C5—H5	0.9800	C26—H26	0.9300
C6—C11	1.360 (6)	C27—H27	0.9300
C6—C7	1.372 (5)	C28—N3	1.432 (5)
C7—C8	1.375 (5)	C28—C29	1.457 (8)
C7—H7	0.9300	C28—C29'	1.539 (10)
C8—C9	1.333 (7)	C28—H28A	0.9700
C8—H8	0.9300	C28—H28B	0.9700
C9—C10	1.333 (8)	C28—H28C	0.9700
C9—H9	0.9300	C28—H28D	0.9700
C10—C11	1.389 (7)	C29—C30	1.500 (9)
C10—H10	0.9300	C29—H29A	0.9700
C11—H11	0.9300	C29—H29B	0.9700
C12—C13	1.375 (4)	C30—C31	1.565 (10)
C12—C17	1.379 (4)	C30—H30A	0.9700
C13—C14	1.386 (4)	C30—H30B	0.9700
C13—H13	0.9300	C31—H31A	0.9600
C14—C15	1.365 (6)	C31—H31B	0.9600
C14—H14	0.9300	C31—H31C	0.9600
C15—C16	1.360 (5)	C29'—C30'	1.535 (10)
C15—H15	0.9300	C29'—H29C	0.9700
C16—C17	1.387 (5)	C29'—H29D	0.9700
C16—H16	0.9300	C30'—C31'	1.522 (10)
C17—H17	0.9300	C30'—H30C	0.9700
C18—C19	1.373 (4)	C30'—H30D	0.9700
C18—C20	1.433 (4)	C31'—H31D	0.9600
C19—N2	1.369 (4)	C31'—H31E	0.9600
C19—S2	1.719 (3)	C31'—H31F	0.9600
C20—O1	1.221 (3)	N3—H3	0.8600
C20—N1	1.423 (4)		
C6—C1—C2	115.0 (2)	C22—C23—C24	119.8 (3)
C6—C1—S1	107.2 (2)	C22—C23—H23	120.1
C2—C1—S1	109.8 (2)	C24—C23—H23	120.1
C6—C1—H1	108.2	C25—C24—C23	118.3 (3)
C2—C1—H1	108.2	C25—C24—H24	120.8
S1—C1—H1	108.2	C23—C24—H24	120.8
C3—C2—C1	112.2 (2)	C24—C25—F1	118.8 (3)
C3—C2—H2A	109.2	C24—C25—C26	123.2 (3)

C1—C2—H2A	109.2	F1—C25—C26	118.0 (3)
C3—C2—H2B	109.2	C25—C26—C27	118.3 (3)
C1—C2—H2B	109.2	C25—C26—H26	120.9
H2A—C2—H2B	107.9	C27—C26—H26	120.9
C4—C3—C18	111.5 (2)	C22—C27—C26	119.6 (3)
C4—C3—C2	123.8 (3)	C22—C27—H27	120.2
C18—C3—C2	124.7 (2)	C26—C27—H27	120.2
C3—C4—C5	129.0 (3)	N3—C28—C29	119.1 (6)
C3—C4—S2	112.4 (2)	N3—C28—C29'	105.3 (7)
C5—C4—S2	118.5 (2)	C29—C28—C29'	29.7 (6)
C4—C5—C12	113.0 (2)	N3—C28—H28A	107.5
C4—C5—S1	111.24 (19)	C29—C28—H28A	107.5
C12—C5—S1	107.9 (2)	C29'—C28—H28A	136.5
C4—C5—H5	108.2	N3—C28—H28B	107.5
C12—C5—H5	108.2	C29—C28—H28B	107.5
S1—C5—H5	108.2	C29'—C28—H28B	89.2
C11—C6—C7	116.4 (4)	H28A—C28—H28B	107.0
C11—C6—C1	120.3 (3)	N3—C28—H28C	110.7
C7—C6—C1	123.2 (3)	C29—C28—H28C	82.1
C6—C7—C8	120.9 (4)	C29'—C28—H28C	111.7
C6—C7—H7	119.6	H28A—C28—H28C	28.6
C8—C7—H7	119.6	H28B—C28—H28C	128.6
C9—C8—C7	121.9 (5)	N3—C28—H28D	111.1
C9—C8—H8	119.0	C29—C28—H28D	120.3
C7—C8—H8	119.0	C29'—C28—H28D	109.1
C10—C9—C8	118.4 (5)	H28A—C28—H28D	84.7
C10—C9—H9	120.8	H28B—C28—H28D	22.8
C8—C9—H9	120.8	H28C—C28—H28D	108.9
C9—C10—C11	121.0 (5)	C28—C29—C30	104.2 (8)
C9—C10—H10	119.5	C28—C29—H29A	110.9
C11—C10—H10	119.5	C30—C29—H29A	110.9
C6—C11—C10	121.3 (5)	C28—C29—H29B	110.9
C6—C11—H11	119.3	C30—C29—H29B	110.9
C10—C11—H11	119.3	H29A—C29—H29B	108.9
C13—C12—C17	118.7 (3)	C29—C30—C31	99.0 (12)
C13—C12—C5	120.8 (2)	C29—C30—H30A	112.0
C17—C12—C5	120.6 (3)	C31—C30—H30A	112.0
C12—C13—C14	120.8 (3)	C29—C30—H30B	112.0
C12—C13—H13	119.6	C31—C30—H30B	112.0
C14—C13—H13	119.6	H30A—C30—H30B	109.6
C15—C14—C13	119.7 (4)	C30'—C29'—C28	119.6 (12)
C15—C14—H14	120.1	C30'—C29'—H29C	107.4
C13—C14—H14	120.1	C28—C29'—H29C	107.4
C16—C15—C14	120.4 (3)	C30'—C29'—H29D	107.4
C16—C15—H15	119.8	C28—C29'—H29D	107.4
C14—C15—H15	119.8	H29C—C29'—H29D	107.0
C15—C16—C17	120.1 (3)	C31'—C30'—C29'	119.9 (18)
C15—C16—H16	120.0	C31'—C30'—H30C	107.4
C17—C16—H16	120.0	C29'—C30'—H30C	107.4

C12—C17—C16	120.4 (3)	C31'—C30'—H30D	107.4
C12—C17—H17	119.8	C29'—C30'—H30D	107.4
C16—C17—H17	119.8	H30C—C30'—H30D	106.9
C19—C18—C20	117.9 (2)	C30'—C31'—H31D	109.5
C19—C18—C3	113.1 (2)	C30'—C31'—H31E	109.5
C20—C18—C3	128.8 (2)	H31D—C31'—H31E	109.5
N2—C19—C18	127.6 (2)	C30'—C31'—H31F	109.5
N2—C19—S2	120.8 (2)	H31D—C31'—H31F	109.5
C18—C19—S2	111.7 (2)	H31E—C31'—H31F	109.5
O1—C20—N1	119.7 (2)	C21—N1—C20	122.8 (2)
O1—C20—C18	126.9 (3)	C21—N1—C22	119.5 (2)
N1—C20—C18	113.3 (2)	C20—N1—C22	117.2 (2)
N2—C21—N3	119.0 (3)	C21—N2—C19	114.1 (2)
N2—C21—N1	123.7 (3)	C21—N3—C28	124.7 (3)
N3—C21—N1	117.3 (2)	C21—N3—H3	117.6
C27—C22—C23	120.8 (3)	C28—N3—H3	117.6
C27—C22—N1	118.4 (2)	C5—S1—C1	99.07 (13)
C23—C22—N1	120.7 (2)	C19—S2—C4	91.32 (13)
C6—C1—C2—C3	−177.7 (3)	C19—C18—C20—N1	−1.5 (3)
S1—C1—C2—C3	−56.7 (3)	C3—C18—C20—N1	−176.3 (2)
C1—C2—C3—C4	22.9 (4)	C27—C22—C23—C24	−0.1 (5)
C1—C2—C3—C18	−155.1 (3)	N1—C22—C23—C24	179.8 (3)
C18—C3—C4—C5	178.1 (3)	C22—C23—C24—C25	−2.2 (5)
C2—C3—C4—C5	−0.1 (4)	C23—C24—C25—F1	−179.0 (3)
C18—C3—C4—S2	1.8 (3)	C23—C24—C25—C26	2.5 (6)
C2—C3—C4—S2	−176.4 (2)	C24—C25—C26—C27	−0.3 (6)
C3—C4—C5—C12	135.7 (3)	F1—C25—C26—C27	−178.8 (3)
S2—C4—C5—C12	−48.1 (3)	C23—C22—C27—C26	2.2 (5)
C3—C4—C5—S1	14.2 (4)	N1—C22—C27—C26	−177.6 (3)
S2—C4—C5—S1	−169.64 (14)	C25—C26—C27—C22	−2.0 (5)
C2—C1—C6—C11	−136.7 (4)	N3—C28—C29—C30	65.7 (10)
S1—C1—C6—C11	100.8 (4)	C29'—C28—C29—C30	−2.7 (19)
C2—C1—C6—C7	42.4 (4)	C28—C29—C30—C31	168.9 (12)
S1—C1—C6—C7	−80.0 (4)	N3—C28—C29'—C30'	−173.1 (15)
C11—C6—C7—C8	−1.5 (6)	C29—C28—C29'—C30'	−50.5 (16)
C1—C6—C7—C8	179.4 (4)	C28—C29'—C30'—C31'	122 (2)
C6—C7—C8—C9	−0.3 (7)	N2—C21—N1—C20	7.0 (4)
C7—C8—C9—C10	1.3 (9)	N3—C21—N1—C20	−171.5 (3)
C8—C9—C10—C11	−0.6 (10)	N2—C21—N1—C22	−165.4 (3)
C7—C6—C11—C10	2.2 (8)	N3—C21—N1—C22	16.1 (4)
C1—C6—C11—C10	−178.6 (5)	O1—C20—N1—C21	176.9 (2)
C9—C10—C11—C6	−1.2 (10)	C18—C20—N1—C21	−4.7 (3)
C4—C5—C12—C13	−55.5 (4)	O1—C20—N1—C22	−10.5 (3)
S1—C5—C12—C13	67.8 (3)	C18—C20—N1—C22	167.9 (2)
C4—C5—C12—C17	123.5 (3)	C27—C22—N1—C21	74.6 (4)
S1—C5—C12—C17	−113.1 (3)	C23—C22—N1—C21	−105.3 (3)
C17—C12—C13—C14	−0.8 (5)	C27—C22—N1—C20	−98.3 (3)
C5—C12—C13—C14	178.3 (3)	C23—C22—N1—C20	81.8 (3)
C12—C13—C14—C15	0.7 (6)	N3—C21—N2—C19	176.3 (3)

C13—C14—C15—C16	−0.3 (7)	N1—C21—N2—C19	−2.2 (4)
C14—C15—C16—C17	−0.1 (7)	C18—C19—N2—C21	−4.7 (4)
C13—C12—C17—C16	0.5 (5)	S2—C19—N2—C21	175.6 (2)
C5—C12—C17—C16	−178.6 (3)	N2—C21—N3—C28	−1.8 (5)
C15—C16—C17—C12	0.0 (6)	N1—C21—N3—C28	176.8 (4)
C4—C3—C18—C19	−2.4 (3)	C29—C28—N3—C21	75.9 (6)
C2—C3—C18—C19	175.8 (3)	C29'—C28—N3—C21	104.4 (9)
C4—C3—C18—C20	172.6 (3)	C4—C5—S1—C1	−41.1 (2)
C2—C3—C18—C20	−9.2 (4)	C12—C5—S1—C1	−165.49 (19)
C20—C18—C19—N2	6.6 (4)	C6—C1—S1—C5	−170.4 (2)
C3—C18—C19—N2	−177.8 (2)	C2—C1—S1—C5	64.0 (2)
C20—C18—C19—S2	−173.70 (19)	N2—C19—S2—C4	179.0 (2)
C3—C18—C19—S2	2.0 (3)	C18—C19—S2—C4	−0.8 (2)
C19—C18—C20—O1	176.8 (3)	C3—C4—S2—C19	−0.6 (2)
C3—C18—C20—O1	1.9 (4)	C5—C4—S2—C19	−177.4 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N2^{i}	0.98	2.60	3.507 (4)	154

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

Fig. 1

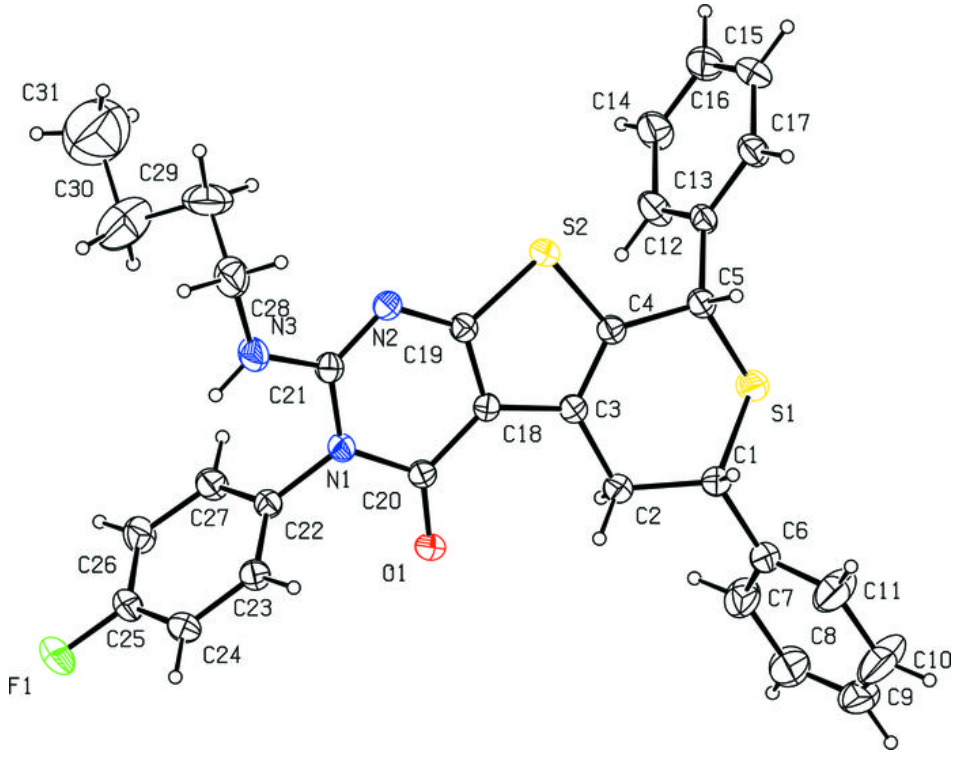
C31
C30
C29
C28
N3
N2
C19
S2
C15
C14
C16
C17
C13
C12
C5
C4
C21
C3
S1
C18
C1
N1
C20
C2
C6
C27
C22
O1
C26
C23
C7
C11
C25
C24
C8
C10
F1
C9

Fig. 2