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5-[(4-Chlorophenyl)diazenyl]-2-[5-(4-fluorophenyl)-3-(furan-2-yl)-4,5-dihydro-1*H*-pyrazol-1-yl]-4-methylthiazole

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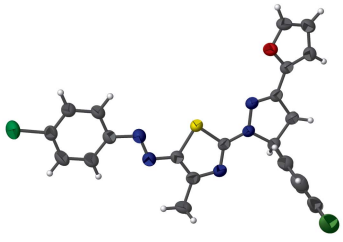
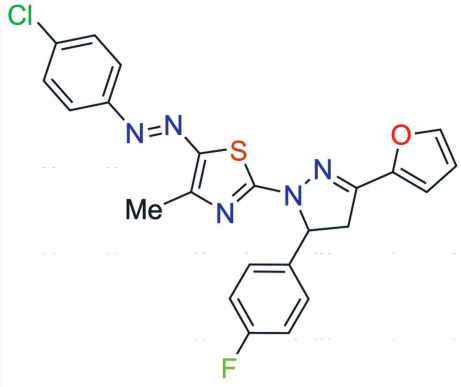
The title compound, $C_{23}H_{17}ClFN_5OS$, comprises fluorophenyl (*A*), furanyl (*B*), pyrazolyl (*C*), methylthiazoyl (*D*) and chlorophenyl (*E*) rings. The *B*–*C*–*D*–*E* linked ring system is close to planar with the dihedral angles *B*/*C*, *C*/*D* and *D*/*E* being 7.6 (1), 3.4 (1) and 8.4 (1)°, respectively. The fluorophenyl group is almost perpendicular to the pyrazoyl ring, as indicated by an *A*/*C* twist angle of 79.4 (1)°. In the crystal, inversion dimers linked by pairs of C—H···S contacts are observed.

3D view



Chemical scheme



Structure description

Thiazoles are of importance in medicinal chemistry as they have various biological activities (Kashyap *et al.*, 2012) and occur in natural products (Chhabria *et al.*, 2016). Pyrazoles have a broad spectrum of biological activities (Faria *et al.*, 2017). As part of our studies in these areas, we now describe the structure of the title compound.

The asymmetric unit consists of one molecule of the title compound and comprises fluorophenyl (*A*), furanyl (*B*), pyrazolyl (*C*), methylthiazoyl (*D*) and chlorophenyl (*E*) rings (Fig. 1). The *B*–*C*–*D*–*E* linked ring system is close to planar with the *B*/*C*, *C*/*D* and *D*/*E* angles between neighbouring rings being 7.6 (1), 3.4 (1) and 8.4 (1)°, respectively. The fluorophenyl group (*A*) is almost perpendicular to the *B*–*E* system as indicated by an

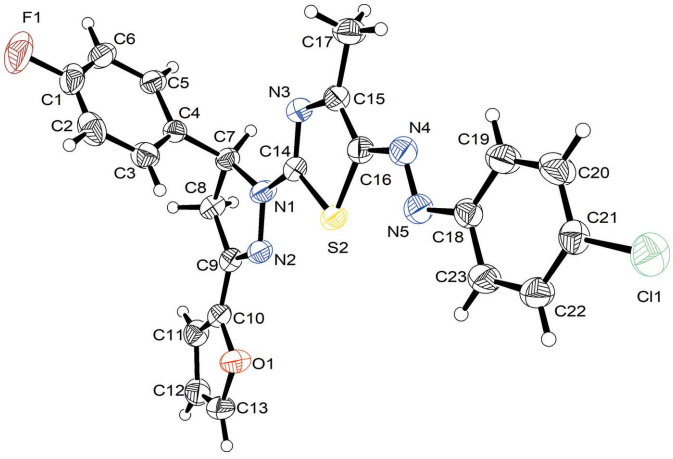


Figure 1
The molecular structure of the title compound showing 50% displacement ellipsoids.

A/*C* twist angle of 79.4 (1)°. In the crystal, inversion dimers linked by pairs of C—H···S bonds (Table 1) generate $R_2^2(18)$ loops, which are stacked in the [100] direction (Fig. 2).

Synthesis and crystallization

The title compound was synthesized by the condensation of 5-(4-fluorophenyl)-3-(furan-2-yl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide with *N*′-(4-chlorophenyl)-2-oxopropanehydrazonoyl chloride in ethanol containing catalytic amount of triethylamine as previously reported (Abdel-Wahab *et al.*, 2013). The product was recrystallized from dimethylformamide solution to give colourless crystals (74%), m.p. 227–228°C.

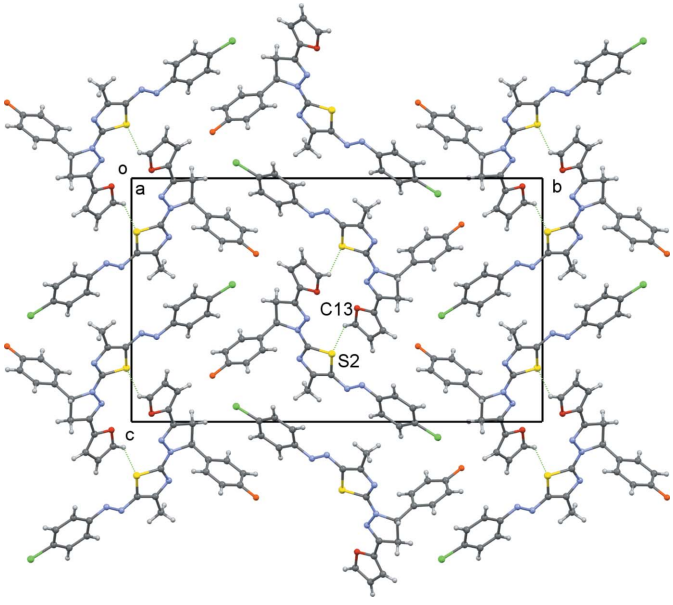


Figure 2
A view of the crystal structure down [100] showing intermolecular short contacts as dotted lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···S2^{i}	0.93	2.85	3.612 (2)	140

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{17}ClFN_5OS$
M_r	465.92
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, *b*, *c* (Å)	5.2879 (3), 26.3742 (10), 15.7872 (7)
β (°)	98.293 (4)
V (Å^3)	2178.72 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.31
Crystal size (mm)	0.49 × 0.16 × 0.15
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.993, 0.997
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21057, 5523, 4143
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.697
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.113, 1.04
No. of reflections	5523
No. of parameters	290
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.31

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXS97* (Sheldrick, 2008), *SHELXL2018* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *CHEMDRAW Ultra* (Cambridge Soft, 2001).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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5-[(4-Chlorophenyl)diazenyl]-2-[5-(4-fluorophenyl)-3-(furan-2-yl)-4,5-dihydro-1*H*-pyrazol-1-yl]-4-methylthiazole

Crystal data

$C_{23}H_{17}ClFN_5OS$
M_r = 465.92
Monoclinic, $P2_1/c$
a = 5.2879 (3) Å
b = 26.3742 (10) Å
c = 15.7872 (7) Å
β = 98.293 (4)°
V = 2178.72 (18) Å^3
Z = 4
$F(000)$ = 960
D_x = 1.420 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6690 reflections
θ = 4.2–28.8°
μ = 0.31 mm^{-1}
T = 298 K
Needle, colourless
0.49 × 0.16 × 0.14 mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, Atlas diffractometer
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.993, T_{max} = 0.997
21057 measured reflections
5523 independent reflections
4143 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 29.7°, θ_{min} = 3.5°
h = −6→6
k = −33→36
l = −18→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 1.03
5523 reflections
290 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.7096P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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. All hydrogen atoms were placed in calculated positions and refined using a riding model. Bond distances for aromatic, methine and methylene C—H hydrogen atoms were set to 0.93 Å, 0.98 Å and 0.93 Å, respectively and their U_{iso} values set to 1.2 times U_{eq}(C). Bond distances for methyl C—H hydrogen atoms were set to 0.96 Å and their U_{iso} set to 1.5 times U_{eq}(C) with the group free to rotate about the C—C bond.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.0781 (5)	0.26438 (8)	0.25920 (13)	0.0626 (6)
C2	−0.0593 (4)	0.22058 (9)	0.25800 (12)	0.0632 (6)
H2	−0.188107	0.216992	0.291921	0.076*
C3	−0.0025 (4)	0.18144 (8)	0.20494 (11)	0.0508 (4)
H3	−0.094947	0.151351	0.202736	0.061*
C4	0.1904 (3)	0.18705 (6)	0.15553 (10)	0.0385 (3)
C5	0.3267 (4)	0.23211 (6)	0.15976 (11)	0.0465 (4)
H5	0.458123	0.235950	0.126987	0.056*
C6	0.2705 (5)	0.27143 (7)	0.21185 (13)	0.0594 (5)
H6	0.361295	0.301722	0.214416	0.071*
C7	0.2489 (3)	0.14657 (6)	0.09325 (11)	0.0414 (4)
H7	0.427871	0.148875	0.084020	0.050*
C8	0.0710 (4)	0.14838 (6)	0.00674 (11)	0.0458 (4)
H8A	−0.030811	0.179117	0.001392	0.055*
H8B	0.167553	0.146253	−0.040917	0.055*
C9	−0.0937 (3)	0.10222 (6)	0.01124 (10)	0.0406 (4)
C10	−0.3123 (4)	0.09025 (6)	−0.05042 (11)	0.0431 (4)
C11	−0.4169 (4)	0.11166 (7)	−0.12524 (11)	0.0510 (4)
H11	−0.358838	0.140346	−0.150784	0.061*
C12	−0.6331 (4)	0.08164 (8)	−0.15704 (12)	0.0559 (5)
H12	−0.743848	0.086687	−0.207690	0.067*
C13	−0.6459 (4)	0.04478 (8)	−0.09992 (13)	0.0568 (5)
H13	−0.770705	0.019689	−0.104760	0.068*
C14	0.3140 (3)	0.07128 (6)	0.19213 (11)	0.0413 (4)
C15	0.5955 (4)	0.05794 (7)	0.30614 (11)	0.0453 (4)
C16	0.4562 (4)	0.01408 (6)	0.30647 (11)	0.0451 (4)
C17	0.8202 (4)	0.07168 (8)	0.37081 (13)	0.0588 (5)
H17A	0.963604	0.079446	0.342109	0.088*
H17B	0.862443	0.043675	0.409091	0.088*
H17C	0.778770	0.100733	0.402770	0.088*
C18	0.3905 (4)	−0.10285 (7)	0.40559 (11)	0.0457 (4)
C19	0.6009 (4)	−0.10844 (8)	0.46822 (13)	0.0598 (5)
H19	0.722638	−0.082798	0.477058	0.072*
C20	0.6311 (4)	−0.15181 (8)	0.51757 (13)	0.0628 (6)
H20	0.772774	−0.155580	0.559425	0.075*

C21	0.4493 (4)	−0.18944 (7)	0.50416 (11)	0.0475 (4)
C22	0.2386 (4)	−0.18456 (7)	0.44334 (12)	0.0565 (5)
H22	0.116268	−0.210100	0.435302	0.068*
C23	0.2105 (4)	−0.14106 (7)	0.39398 (13)	0.0563 (5)
H23	0.068133	−0.137504	0.352340	0.068*
N1	0.1930 (3)	0.09521 (5)	0.12251 (9)	0.0466 (4)
N2	−0.0195 (3)	0.07306 (5)	0.07564 (9)	0.0444 (3)
N3	0.5145 (3)	0.09084 (5)	0.24081 (9)	0.0452 (3)
N4	0.5021 (3)	−0.02481 (6)	0.36380 (9)	0.0480 (4)
N5	0.3409 (3)	−0.06088 (6)	0.34945 (10)	0.0503 (4)
F1	0.0203 (4)	0.30294 (6)	0.31041 (9)	0.1010 (6)
S2	0.20523 (9)	0.01261 (2)	0.22069 (3)	0.04565 (13)
Cl1	0.49098 (13)	−0.24529 (2)	0.56357 (3)	0.07087 (18)
O1	−0.4519 (3)	0.04886 (5)	−0.03373 (8)	0.0550 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0723 (15)	0.0617 (12)	0.0474 (10)	0.0251 (11)	−0.0127 (10)	−0.0170 (9)
C2	0.0544 (13)	0.0884 (16)	0.0475 (10)	0.0187 (11)	0.0095 (9)	−0.0047 (10)
C3	0.0451 (11)	0.0570 (11)	0.0504 (10)	−0.0036 (8)	0.0076 (8)	−0.0034 (8)
C4	0.0371 (9)	0.0372 (8)	0.0398 (8)	−0.0012 (6)	0.0012 (6)	0.0004 (6)
C5	0.0482 (11)	0.0399 (9)	0.0491 (9)	−0.0048 (7)	−0.0007 (8)	0.0001 (7)
C6	0.0702 (15)	0.0404 (10)	0.0604 (12)	0.0013 (9)	−0.0152 (10)	−0.0079 (8)
C7	0.0424 (10)	0.0352 (8)	0.0473 (9)	−0.0052 (7)	0.0087 (7)	−0.0015 (7)
C8	0.0553 (11)	0.0403 (9)	0.0417 (9)	−0.0062 (8)	0.0071 (8)	−0.0021 (7)
C9	0.0450 (10)	0.0357 (8)	0.0416 (8)	−0.0002 (7)	0.0078 (7)	−0.0031 (6)
C10	0.0469 (10)	0.0380 (8)	0.0445 (9)	−0.0023 (7)	0.0073 (7)	−0.0038 (7)
C11	0.0572 (12)	0.0473 (10)	0.0472 (9)	0.0034 (8)	0.0035 (8)	0.0022 (8)
C12	0.0574 (13)	0.0578 (11)	0.0486 (10)	0.0084 (9)	−0.0050 (9)	−0.0065 (8)
C13	0.0500 (12)	0.0548 (11)	0.0613 (11)	−0.0068 (9)	−0.0066 (9)	−0.0083 (9)
C14	0.0432 (10)	0.0344 (8)	0.0460 (9)	0.0005 (7)	0.0048 (7)	−0.0042 (7)
C15	0.0430 (10)	0.0462 (9)	0.0460 (9)	0.0013 (7)	0.0038 (7)	−0.0081 (7)
C16	0.0466 (10)	0.0436 (9)	0.0434 (9)	0.0026 (7)	0.0007 (7)	−0.0034 (7)
C17	0.0512 (12)	0.0675 (13)	0.0543 (11)	−0.0070 (10)	−0.0043 (9)	−0.0089 (9)
C18	0.0461 (11)	0.0468 (9)	0.0428 (9)	0.0037 (8)	0.0013 (7)	0.0001 (7)
C19	0.0511 (12)	0.0591 (12)	0.0647 (12)	−0.0075 (9)	−0.0071 (9)	0.0090 (9)
C20	0.0536 (13)	0.0695 (13)	0.0588 (11)	−0.0006 (10)	−0.0136 (9)	0.0128 (10)
C21	0.0543 (12)	0.0478 (9)	0.0399 (8)	0.0058 (8)	0.0054 (8)	0.0036 (7)
C22	0.0565 (13)	0.0495 (10)	0.0592 (11)	−0.0059 (9)	−0.0066 (9)	0.0042 (8)
C23	0.0532 (12)	0.0534 (11)	0.0559 (11)	−0.0018 (9)	−0.0138 (9)	0.0042 (8)
N1	0.0522 (9)	0.0332 (7)	0.0506 (8)	−0.0070 (6)	−0.0060 (7)	0.0001 (6)
N2	0.0472 (9)	0.0367 (7)	0.0469 (8)	−0.0040 (6)	−0.0011 (6)	−0.0018 (6)
N3	0.0457 (9)	0.0403 (7)	0.0485 (8)	−0.0033 (6)	0.0024 (6)	−0.0046 (6)
N4	0.0510 (10)	0.0463 (8)	0.0456 (8)	0.0020 (7)	0.0030 (7)	−0.0001 (6)
N5	0.0530 (10)	0.0462 (8)	0.0493 (8)	0.0020 (7)	−0.0006 (7)	0.0027 (6)
F1	0.1302 (14)	0.0924 (10)	0.0740 (9)	0.0464 (10)	−0.0072 (9)	−0.0408 (8)
S2	0.0486 (3)	0.0353 (2)	0.0500 (2)	−0.00246 (17)	−0.00321 (19)	−0.00071 (16)

Cl1	0.0867 (4)	0.0649 (3)	0.0580 (3)	0.0043 (3)	0.0002 (3)	0.0203 (2)
O1	0.0565 (9)	0.0499 (7)	0.0546 (7)	−0.0141 (6)	−0.0052 (6)	0.0049 (6)

Geometric parameters (Å, º)

C1—C6	1.359 (3)	C13—H13	0.9300
C1—F1	1.361 (2)	C14—N3	1.321 (2)
C1—C2	1.363 (3)	C14—N1	1.346 (2)
C2—C3	1.389 (3)	C14—S2	1.7330 (17)
C2—H2	0.9300	C15—N3	1.369 (2)
C3—C4	1.379 (2)	C15—C16	1.372 (3)
C3—H3	0.9300	C15—C17	1.495 (3)
C4—C5	1.386 (2)	C16—N4	1.366 (2)
C4—C7	1.513 (2)	C16—S2	1.7546 (18)
C5—C6	1.382 (3)	C17—H17A	0.9600
C5—H5	0.9300	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C7—N1	1.475 (2)	C18—C23	1.380 (3)
C7—C8	1.543 (2)	C18—C19	1.386 (3)
C7—H7	0.9800	C18—N5	1.419 (2)
C8—C9	1.504 (2)	C19—C20	1.380 (3)
C8—H8A	0.9700	C19—H19	0.9300
C8—H8B	0.9700	C20—C21	1.377 (3)
C9—N2	1.290 (2)	C20—H20	0.9300
C9—C10	1.435 (2)	C21—C22	1.368 (3)
C10—C11	1.353 (2)	C21—Cl1	1.7432 (18)
C10—O1	1.365 (2)	C22—C23	1.383 (3)
C11—C12	1.422 (3)	C22—H22	0.9300
C11—H11	0.9300	C23—H23	0.9300
C12—C13	1.334 (3)	N1—N2	1.3823 (19)
C12—H12	0.9300	N4—N5	1.276 (2)
C13—O1	1.359 (2)		
C6—C1—F1	118.3 (2)	O1—C13—H13	124.6
C6—C1—C2	123.24 (18)	N3—C14—N1	122.60 (15)
F1—C1—C2	118.4 (2)	N3—C14—S2	117.77 (13)
C1—C2—C3	118.5 (2)	N1—C14—S2	119.63 (13)
C1—C2—H2	120.8	N3—C15—C16	115.32 (16)
C3—C2—H2	120.8	N3—C15—C17	119.51 (16)
C4—C3—C2	120.21 (19)	C16—C15—C17	125.17 (17)
C4—C3—H3	119.9	N4—C16—C15	126.26 (17)
C2—C3—H3	119.9	N4—C16—S2	122.47 (14)
C3—C4—C5	119.12 (16)	C15—C16—S2	111.26 (13)
C3—C4—C7	121.94 (15)	C15—C17—H17A	109.5
C5—C4—C7	118.85 (15)	C15—C17—H17B	109.5
C6—C5—C4	121.13 (19)	H17A—C17—H17B	109.5
C6—C5—H5	119.4	C15—C17—H17C	109.5
C4—C5—H5	119.4	H17A—C17—H17C	109.5

C1—C6—C5	117.82 (19)	H17B—C17—H17C	109.5
C1—C6—H6	121.1	C23—C18—C19	118.99 (17)
C5—C6—H6	121.1	C23—C18—N5	115.16 (16)
N1—C7—C4	112.05 (14)	C19—C18—N5	125.85 (17)
N1—C7—C8	100.45 (13)	C20—C19—C18	120.42 (19)
C4—C7—C8	113.43 (14)	C20—C19—H19	119.8
N1—C7—H7	110.2	C18—C19—H19	119.8
C4—C7—H7	110.2	C21—C20—C19	119.30 (18)
C8—C7—H7	110.2	C21—C20—H20	120.4
C9—C8—C7	102.49 (13)	C19—C20—H20	120.4
C9—C8—H8A	111.3	C22—C21—C20	121.34 (17)
C7—C8—H8A	111.3	C22—C21—Cl1	118.96 (15)
C9—C8—H8B	111.3	C20—C21—Cl1	119.67 (15)
C7—C8—H8B	111.3	C21—C22—C23	118.96 (18)
H8A—C8—H8B	109.2	C21—C22—H22	120.5
N2—C9—C10	121.82 (15)	C23—C22—H22	120.5
N2—C9—C8	114.04 (15)	C18—C23—C22	120.99 (18)
C10—C9—C8	124.13 (15)	C18—C23—H23	119.5
C11—C10—O1	109.75 (16)	C22—C23—H23	119.5
C11—C10—C9	133.48 (17)	C14—N1—N2	119.53 (14)
O1—C10—C9	116.77 (15)	C14—N1—C7	126.37 (14)
C10—C11—C12	106.40 (17)	N2—N1—C7	113.86 (13)
C10—C11—H11	126.8	C9—N2—N1	107.54 (14)
C12—C11—H11	126.8	C14—N3—C15	109.17 (14)
C13—C12—C11	106.48 (17)	N5—N4—C16	113.09 (15)
C13—C12—H12	126.8	N4—N5—C18	114.36 (15)
C11—C12—H12	126.8	C14—S2—C16	86.48 (8)
C12—C13—O1	110.85 (17)	C13—O1—C10	106.51 (14)
C12—C13—H13	124.6		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13···S2^{i}	0.93	2.85	3.612 (2)	140

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