



# Crystal structure and Hirshfeld surface analysis of 1-(4-chlorophenyl)-2-[[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]sulfanyl]ethanone

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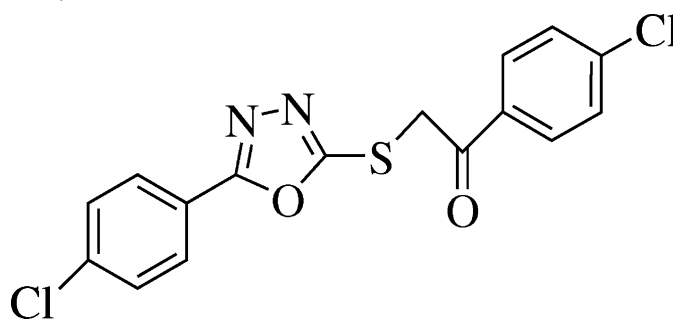
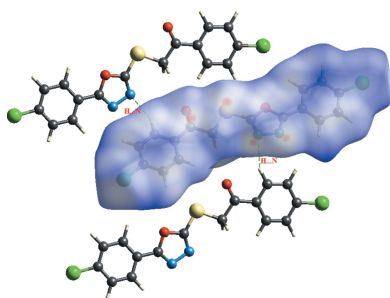
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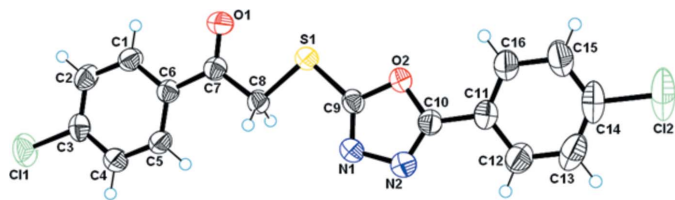
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In the title compound, C<sub>16</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>S, the dihedral angles formed by the chloro-substituted benzene rings with the central oxadiazole ring are 6.54 (9) and 6.94 (8)°. In the crystal, C—H···N hydrogen bonding links the molecules into undulating ribbons running parallel to the *b* axis. Hirshfeld surface analysis indicates that the most important contributions for the crystal packing are the H···C (18%), H···H (17%), H···Cl (16.6%), H···O (10.4%), H···N (8.9%) and H···S (5.9%) interactions.

## 1. Chemical context

Heterocyclic compounds are well known for their applications in agriculture (Jakobi *et al.*, 1999) and for the synthesis of pharmaceuticals (Vitaku *et al.*, 2014). The broad range of biological activities of heterocyclic compounds has always fascinated chemists and the literature reveals many approaches to synthesize and derivatize libraries of heterocyclic compounds (Khan *et al.*, 2011; Chohan *et al.*, 2006; Khan *et al.*, 2005). The wide range of applications and biological activities of this class of compounds is due to the presence of heteroatoms (N, O, S) in the molecule (Kashtoh *et al.*, 2014). Oxadiazoles are among the most widely studied moieties of organic chemistry due to their many important chemical and biological properties including antimycobacterial (Jha *et al.*, 2009), antioxidant (Fadda *et al.*, 2011), anticancer (Zhang *et al.*, 2011), antitumor (Loetchutinat *et al.*, 2003), antimicrobial (Şahin *et al.*, 2002), antifungal (Zou *et al.*, 2002), anti-inflammatory (Palaska *et al.*, 2002) and hypotensive (Tyagi & Kumar, 2002) activities.





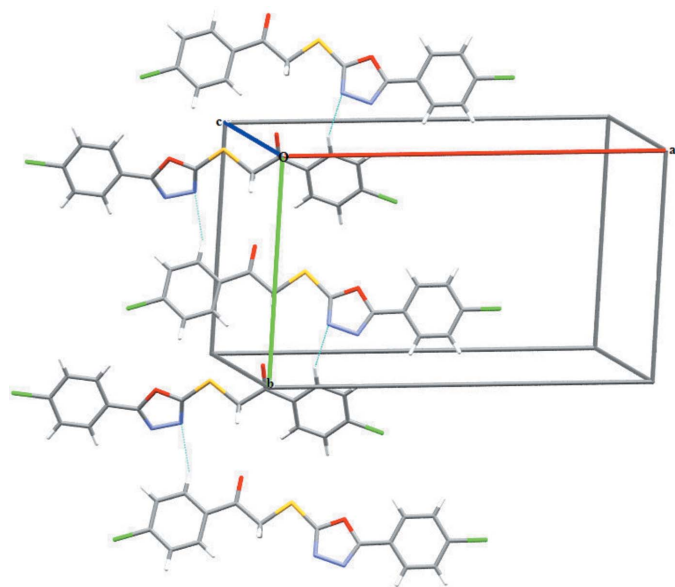
**Figure 1**  
The molecular structure of the title compound with displacement ellipsoids drawn at 30% probability level.

## 2. Structural commentary

The title compound (Fig. 1) is an oxadiazole derivative containing two chlorophenyl substituents attached to a central oxadiazole thioethanone unit. The C1–C6 and C11–C16 phenyl rings form dihedral angles of 6.54 (9) and 6.94 (8)°, respectively, with the oxadiazole ring. The dihedral angle between the oxadiazole ring and the mean plane through the S1/O1/C7–C8 fragment is 10.75 (8)°. Bond lengths and angles are not unusual.

## 3. Supramolecular features

In the crystal, molecules are connected by C–H···N hydrogen interactions, forming undulating ribbons parallel to the *b* axis (Table 1, Fig. 2). The importance of these interactions in stabilizing the crystal structure may be determined by comparison with those found in similar related compounds. For instance, in the crystal structure of 2-[5-[(1*H*-1,2,4-triazol-1-yl)methyl]-1,3,4-oxadiazol-2-ylthio]-1-(2,4-dichlorophenyl) ethanone (Xu *et al.*, 2005) molecules are linked into chains *via*



**Figure 2**  
Partial crystal packing of the title compound showing the formation of an undulating ribbon parallel to the *b* axis through C–H···N hydrogen bonds (dashed lines).

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

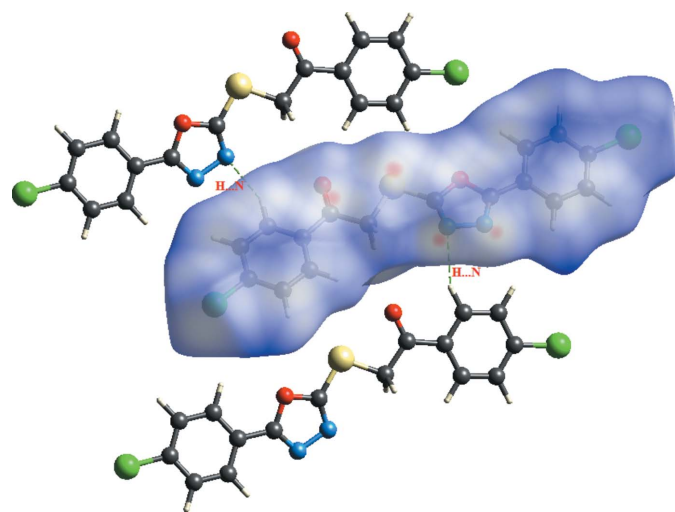
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C1–H1 <i>B</i> ···N1 <sup>i</sup>	0.93	2.48	3.353 (3)	157

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

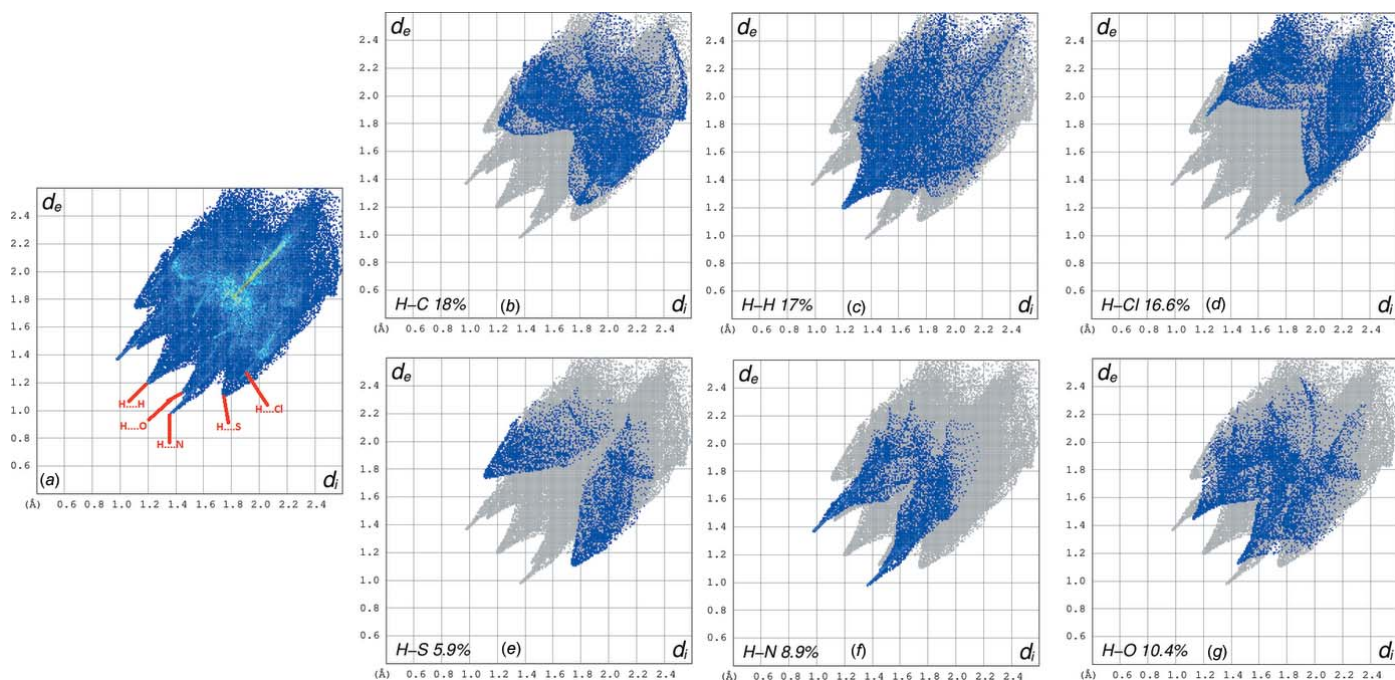
C–H···N hydrogen bonds having H···N separations of 2.48 Å and C–H···C interactions having H···N distances of 2.41 Å. Similarly, in the crystal structure of 1,3-*bis*[[5-(pyridin-2-yl)-1,3,4-oxadiazol-2-yl]sulfanyl]propan-2-one (Xia *et al.*, 2011), two oxadiazole rings are present and form intermolecular hydrogen bonds of the type C–H···N with distances of 2.51 and 2.54 Å, respectively. Moreover, in the structure of the latter compound, further stabilization of the crystal structure is provided by  $\pi$ – $\pi$  interactions involving the pyridyl and oxadiazole rings with centroid-to-centroid distances of 3.883 Å.

## 4. Hirshfeld surface analysis

The Hirshfeld surface analysis (Spackman & Jayatilaka, 2009) of the crystal structure suggests that the contribution to the crystal packing of the H···N interaction is 8.9% (Fig. 3). Other important interactions based upon the percentages are H···H (17%), H···O (10.4%), H···C (18%), H···S (5.9%) and H···Cl (16.6%). These interactions, however, were not found to be involved in hydrogen bonding, as observed for the H···N contribution (Fig. 4). The Hirshfeld surface diagram shows the location of atoms with the potential to form hydrogen bonds. These interactions are represented in two-dimensional fingerprint plots (Fig. 4), in which the cyan dots indicate the percentage of the interaction over the total Hirshfeld surface.



**Figure 3**  
 $d_{\text{norm}}$  mapped on the Hirshfeld surface, visualizing the intermolecular contacts of the title compound. Dotted lines indicate hydrogen bonds.



**Figure 4** Hirshfeld surface two-dimensional fingerprint plot for the title compound (a) showing the: (b) H...C, (c) H...H, (d) H...Cl, (e) H...S, (f) H...N and (g) H...O interactions. The outline of the full fingerprint plots is shown in gray.  $d_i$  (x axis) and  $d_e$  (y axis) are the closest internal and external distance (values in Å) from a given point on the Hirshfeld surface contacts.

## 5. Synthesis and crystallization

The title compound was synthesized by the procedure reported by Kashtoh *et al.* (2014). 4-Chloro-1,3,4-oxadiazole-2-thiol (212 mg, 1 mmol) and triethyl amine (0.1 mL) were taken in ethanol (10 mL) and stirred for 10 min. 2-Bromo-4'-chloroacetophenone (232 mg, 1 mmol) was then added slowly into the mixture and refluxed, while progress of the reaction was monitored by TLC. After completion of the reaction, the precipitate was filtered and washed with ethanol. The precipitate was crystallized from methanol to give the title compound in 344 mg, 94% yield.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in (Table 2). H atoms were located in a difference-Fourier map, but were positioned with idealized geometry and refined with C–H = 0.93–0.97 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Funding information

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**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{16}\text{H}_{10}\text{Cl}_2\text{N}_2\text{O}_2\text{S}$
$M_r$	365.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	273
$a, b, c$ (Å)	19.1513 (7), 11.1589 (4), 7.5071 (3)
$\beta$ (°)	92.088 (1)
$V$ (Å <sup>3</sup> )	1603.26 (10)
$Z$	4
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.55
Crystal size (mm)	0.47 × 0.39 × 0.11
Data collection	
Diffractometer	Bruker <i>SMART APEX</i> CCD area-detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2000)
$T_{\text{min}}, T_{\text{max}}$	0.784, 0.945
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	11526, 3762, 3058
$R_{\text{int}}$	0.022
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.045, 0.132, 1.12
No. of reflections	3762
No. of parameters	208
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.34, -0.26

Computer programs: *SMART* and *SAINT* (Bruker, 2000), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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## supporting information

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### Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

### 1-(4-Chlorophenyl)-2-[[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]sulfanyl]ethanone

#### Crystal data

$C_{16}H_{10}Cl_2N_2O_2S$   
 $M_r = 365.22$   
 Monoclinic,  $P2_1/c$   
 $a = 19.1513$  (7) Å  
 $b = 11.1589$  (4) Å  
 $c = 7.5071$  (3) Å  
 $\beta = 92.088$  (1)°  
 $V = 1603.26$  (10) Å<sup>3</sup>  
 $Z = 4$

$F(000) = 744$   
 $D_x = 1.513$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å  
 Cell parameters from 3559 reflections  
 $\theta = 3.2$ – $27.7$ °  
 $\mu = 0.55$  mm<sup>-1</sup>  
 $T = 273$  K  
 Block, colorless  
 $0.47 \times 0.39 \times 0.11$  mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scan  
 Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.784$ ,  $T_{\max} = 0.945$

11526 measured reflections  
 3762 independent reflections  
 3058 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$   
 $\theta_{\text{max}} = 28.3$ °,  $\theta_{\text{min}} = 1.1$ °  
 $h = -25 \rightarrow 25$   
 $k = -13 \rightarrow 14$   
 $l = -9 \rightarrow 9$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.132$   
 $S = 1.12$   
 3762 reflections  
 208 parameters  
 0 restraints  
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map  
 Hydrogen site location: inferred from neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.2639P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.34$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	−0.31166 (3)	0.71345 (7)	0.43607 (10)	0.0711 (2)
C12	0.54160 (4)	0.62796 (12)	−0.30547 (16)	0.1258 (4)
S1	0.09911 (2)	0.52100 (4)	0.14177 (7)	0.04411 (16)
O1	−0.01151 (8)	0.43467 (13)	0.3026 (2)	0.0556 (4)
O2	0.21861 (7)	0.57741 (12)	0.00900 (19)	0.0427 (3)
N1	0.14210 (9)	0.72473 (14)	−0.0287 (2)	0.0457 (4)
N2	0.20649 (9)	0.75906 (16)	−0.1028 (3)	0.0508 (4)
C1	−0.14356 (11)	0.50990 (18)	0.3877 (3)	0.0448 (5)
H1B	−0.1303	0.4313	0.4130	0.054*
C2	−0.20957 (11)	0.54753 (19)	0.4258 (3)	0.0494 (5)
H2B	−0.2410	0.4953	0.4766	0.059*
C3	−0.22851 (10)	0.6646 (2)	0.3873 (3)	0.0463 (5)
C4	−0.18228 (10)	0.74359 (19)	0.3131 (3)	0.0471 (5)
H4A	−0.1958	0.8222	0.2889	0.057*
C5	−0.11620 (10)	0.70548 (17)	0.2752 (3)	0.0428 (4)
H5A	−0.0849	0.7583	0.2250	0.051*
C6	−0.09600 (9)	0.58753 (16)	0.3118 (3)	0.0375 (4)
C7	−0.02636 (10)	0.53891 (16)	0.2705 (3)	0.0394 (4)
C8	0.02691 (9)	0.61879 (16)	0.1858 (3)	0.0410 (4)
H8A	0.0415	0.6828	0.2663	0.049*
H8B	0.0079	0.6537	0.0761	0.049*
C9	0.15279 (9)	0.61954 (16)	0.0337 (3)	0.0385 (4)
C10	0.24856 (10)	0.67088 (18)	−0.0775 (3)	0.0419 (4)
C11	0.32086 (10)	0.6589 (2)	−0.1300 (3)	0.0466 (5)
C12	0.35671 (13)	0.7597 (2)	−0.1857 (3)	0.0611 (6)
H12A	0.3347	0.8340	−0.1876	0.073*
C13	0.42443 (14)	0.7499 (3)	−0.2380 (4)	0.0743 (8)
H13A	0.4485	0.8174	−0.2747	0.089*
C14	0.45624 (12)	0.6400 (3)	−0.2356 (4)	0.0760 (8)
C15	0.42210 (13)	0.5394 (3)	−0.1805 (5)	0.0819 (9)
H15A	0.4444	0.4654	−0.1793	0.098*
C16	0.35398 (12)	0.5494 (2)	−0.1265 (4)	0.0643 (7)
H16A	0.3305	0.4818	−0.0877	0.077*



*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	0.0415 (3)	0.0839 (5)	0.0889 (5)	0.0064 (3)	0.0182 (3)	-0.0073 (3)
C12	0.0440 (4)	0.1827 (11)	0.1531 (10)	-0.0066 (5)	0.0351 (5)	0.0047 (8)
S1	0.0393 (3)	0.0369 (3)	0.0567 (4)	0.00321 (18)	0.0088 (2)	0.0004 (2)
O1	0.0519 (8)	0.0395 (8)	0.0761 (11)	0.0055 (6)	0.0118 (7)	0.0083 (7)
O2	0.0347 (6)	0.0408 (7)	0.0531 (9)	0.0030 (5)	0.0068 (6)	0.0007 (6)
N1	0.0402 (8)	0.0399 (9)	0.0575 (11)	0.0064 (7)	0.0061 (7)	0.0015 (7)
N2	0.0464 (9)	0.0448 (9)	0.0615 (12)	0.0013 (8)	0.0073 (8)	0.0058 (8)
C1	0.0474 (11)	0.0396 (10)	0.0477 (12)	-0.0031 (8)	0.0055 (9)	0.0040 (8)
C2	0.0458 (11)	0.0505 (12)	0.0527 (13)	-0.0098 (9)	0.0122 (9)	0.0030 (9)
C3	0.0349 (9)	0.0569 (12)	0.0472 (12)	-0.0011 (8)	0.0050 (8)	-0.0066 (9)
C4	0.0446 (11)	0.0421 (10)	0.0550 (13)	0.0043 (8)	0.0053 (9)	-0.0002 (9)
C5	0.0415 (10)	0.0385 (10)	0.0488 (12)	-0.0034 (7)	0.0067 (8)	0.0025 (8)
C6	0.0376 (9)	0.0369 (9)	0.0380 (11)	-0.0020 (7)	0.0025 (7)	-0.0035 (7)
C7	0.0407 (9)	0.0384 (10)	0.0393 (11)	-0.0018 (7)	0.0024 (8)	-0.0039 (7)
C8	0.0349 (9)	0.0374 (10)	0.0511 (12)	-0.0001 (7)	0.0062 (8)	-0.0050 (8)
C9	0.0341 (9)	0.0387 (9)	0.0428 (11)	0.0023 (7)	0.0020 (7)	-0.0067 (8)
C10	0.0387 (9)	0.0428 (10)	0.0441 (12)	-0.0009 (8)	0.0022 (8)	-0.0023 (8)
C11	0.0380 (10)	0.0553 (12)	0.0466 (12)	-0.0055 (8)	0.0017 (8)	-0.0023 (9)
C12	0.0542 (13)	0.0643 (14)	0.0652 (16)	-0.0073 (11)	0.0064 (11)	0.0097 (12)
C13	0.0563 (15)	0.094 (2)	0.0731 (19)	-0.0240 (15)	0.0099 (12)	0.0140 (15)
C14	0.0358 (11)	0.115 (2)	0.0776 (19)	-0.0088 (13)	0.0123 (11)	-0.0057 (16)
C15	0.0443 (13)	0.0813 (19)	0.121 (3)	0.0050 (12)	0.0181 (14)	-0.0089 (17)
C16	0.0429 (11)	0.0570 (13)	0.0939 (19)	-0.0010 (10)	0.0144 (12)	-0.0044 (13)

*Geometric parameters (Å, °)*

C11—C3	1.735 (2)	C5—C6	1.396 (3)
C12—C14	1.740 (2)	C5—H5A	0.9300
S1—C9	1.7279 (19)	C6—C7	1.483 (2)
S1—C8	1.8014 (18)	C7—C8	1.512 (2)
O1—C7	1.219 (2)	C8—H8A	0.9700
O2—C9	1.364 (2)	C8—H8B	0.9700
O2—C10	1.366 (2)	C10—C11	1.459 (3)
N1—C9	1.277 (2)	C11—C16	1.376 (3)
N1—N2	1.424 (2)	C11—C12	1.390 (3)
N2—C10	1.281 (3)	C12—C13	1.373 (3)
C1—C2	1.372 (3)	C12—H12A	0.9300
C1—C6	1.394 (3)	C13—C14	1.369 (4)
C1—H1B	0.9300	C13—H13A	0.9300
C2—C3	1.384 (3)	C14—C15	1.370 (4)
C2—H2B	0.9300	C15—C16	1.385 (3)
C3—C4	1.381 (3)	C15—H15A	0.9300
C4—C5	1.375 (3)	C16—H16A	0.9300
C4—H4A	0.9300		

C9—S1—C8	100.05 (9)	C7—C8—H8B	110.8
C9—O2—C10	101.97 (14)	S1—C8—H8B	110.8
C9—N1—N2	105.12 (15)	H8A—C8—H8B	108.9
C10—N2—N1	106.51 (16)	N1—C9—O2	113.80 (16)
C2—C1—C6	121.04 (18)	N1—C9—S1	131.81 (14)
C2—C1—H1B	119.5	O2—C9—S1	114.39 (13)
C6—C1—H1B	119.5	N2—C10—O2	112.59 (17)
C1—C2—C3	118.81 (18)	N2—C10—C11	128.91 (19)
C1—C2—H2B	120.6	O2—C10—C11	118.50 (17)
C3—C2—H2B	120.6	C16—C11—C12	119.5 (2)
C4—C3—C2	121.32 (18)	C16—C11—C10	121.17 (19)
C4—C3—C11	119.47 (17)	C12—C11—C10	119.4 (2)
C2—C3—C11	119.20 (16)	C13—C12—C11	120.2 (3)
C5—C4—C3	119.66 (19)	C13—C12—H12A	119.9
C5—C4—H4A	120.2	C11—C12—H12A	119.9
C3—C4—H4A	120.2	C14—C13—C12	119.5 (2)
C4—C5—C6	120.09 (18)	C14—C13—H13A	120.3
C4—C5—H5A	120.0	C12—C13—H13A	120.3
C6—C5—H5A	120.0	C13—C14—C15	121.4 (2)
C1—C6—C5	119.08 (17)	C13—C14—C12	119.2 (2)
C1—C6—C7	117.65 (17)	C15—C14—C12	119.4 (2)
C5—C6—C7	123.26 (17)	C14—C15—C16	119.2 (3)
O1—C7—C6	120.85 (17)	C14—C15—H15A	120.4
O1—C7—C8	119.29 (17)	C16—C15—H15A	120.4
C6—C7—C8	119.85 (16)	C11—C16—C15	120.3 (2)
C7—C8—S1	104.72 (12)	C11—C16—H16A	119.9
C7—C8—H8A	110.8	C15—C16—H16A	119.9
S1—C8—H8A	110.8		
C9—N1—N2—C10	0.2 (2)	C10—O2—C9—S1	179.80 (13)
C6—C1—C2—C3	0.1 (3)	C8—S1—C9—N1	-11.3 (2)
C1—C2—C3—C4	-0.5 (3)	C8—S1—C9—O2	169.15 (14)
C1—C2—C3—C11	-179.61 (17)	N1—N2—C10—O2	-0.1 (2)
C2—C3—C4—C5	0.5 (3)	N1—N2—C10—C11	179.0 (2)
C11—C3—C4—C5	179.62 (16)	C9—O2—C10—N2	0.0 (2)
C3—C4—C5—C6	-0.1 (3)	C9—O2—C10—C11	-179.28 (17)
C2—C1—C6—C5	0.3 (3)	N2—C10—C11—C16	-166.0 (2)
C2—C1—C6—C7	-178.44 (19)	O2—C10—C11—C16	13.1 (3)
C4—C5—C6—C1	-0.3 (3)	N2—C10—C11—C12	13.5 (4)
C4—C5—C6—C7	178.38 (18)	O2—C10—C11—C12	-167.4 (2)
C1—C6—C7—O1	-0.2 (3)	C16—C11—C12—C13	0.5 (4)
C5—C6—C7—O1	-178.9 (2)	C10—C11—C12—C13	-179.1 (2)
C1—C6—C7—C8	179.18 (17)	C11—C12—C13—C14	0.3 (4)
C5—C6—C7—C8	0.5 (3)	C12—C13—C14—C15	-0.6 (5)
O1—C7—C8—S1	4.4 (2)	C12—C13—C14—C12	179.0 (2)
C6—C7—C8—S1	-174.98 (14)	C13—C14—C15—C16	0.1 (5)
C9—S1—C8—C7	176.28 (13)	C12—C14—C15—C16	-179.4 (2)
N2—N1—C9—O2	-0.2 (2)	C12—C11—C16—C15	-0.9 (4)



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N2—N1—C9—S1	-179.78 (16)	C10—C11—C16—C15	178.6 (2)
C10—O2—C9—N1	0.2 (2)	C14—C15—C16—C11	0.6 (5)

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*Hydrogen-bond geometry (Å, °)*

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C1—H1 <i>B</i> ···N1 <sup>i</sup>	0.93	2.48	3.353 (3)	157

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