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ISSN 2414-3146

3-(2,5-Dichlorothiophen-3-yl)-5-(2,4-dimethoxyphenyl)-1-methyl-4,5-dihydro-1*H*-pyrazole

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Received 19 July 2019
Accepted 23 July 2019

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

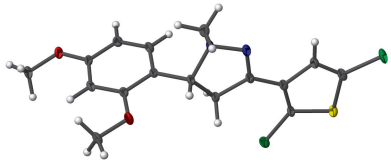
Keywords: crystal structure; pyrazole; Cl···π interactions.

CCDC reference: 1906405

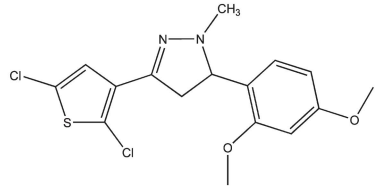
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{16}Cl_2N_2O_2S$, the pyrazole ring has an envelope conformation with the C atom bearing the phenyl ring being the flap. The dihedral angles between the central pyrazole ring (all atoms) and pendant thiophene and phenyl rings are 2.00 (14) and 81.49 (12)°, respectively. In the crystal, weak C—H···O, Cl···π and π–π stacking interactions link the molecules into a three-dimensional network.

3D view



Chemical scheme



Structure description

Heterocyclic compounds containing a pyrazole core show various biological properties such as anti-cancer (Sidique *et al.*, 2009), anti-inflammatory (Viveka *et al.*, 2015) and antioxidant activities (Taj *et al.*, 2011). In a continuation of our ongoing research on pyrazoles (Ibrahim *et al.*, 2016), we now describe the synthesis and structure of the title compound, **I** (Fig. 1).

The central pyrazole ring adopts an envelope conformation with the chiral C3 atom as the flap [deviation from the other atoms = 0.363 (3) Å]. C3 has an *R* configuration in the arbitrarily chosen asymmetric unit but crystal symmetry generates a racemic mixture. The C atom of the methyl group attached to N2 of the pyrazole ring deviates significantly by 0.758 (3) Å from the plane of N1/N2/C4/C5 (r.m.s. deviation = 0.025 Å), which suggests that the electronic structure of N2 is well described as being sp^3 hybridized.

The thiophene ring at position C5, and the phenyl ring at position C3 are inclined to the pyrazole ring (all atoms) by dihedral angles of 2.00 (14) and 81.49 (12)°, respectively; the dihedral angle between the pendant rings is 82.76 (11)°. The C atoms of the methoxy groups lie close to the plane of the phenyl ring [deviations for C18 and C19 = −0.081 (2) and 0.045 (2) Å, respectively]. The molecular structure features a short intramolecular C3—H3···O1 contact of 2.39 Å (Table 1), which closes an *S*(5) ring.

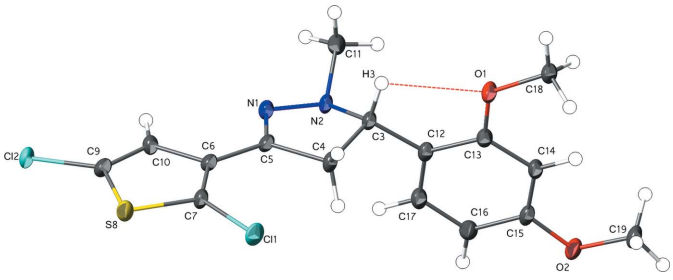


Figure 1
The molecular structure of **I** (50% probability displacement ellipsoids) with the short C—H···O interaction shown as a dashed line.

The extended structure of **I** (Fig. 2) features very weak C11—H11*C*···O2(x, $-1+y$, z) hydrogen bonds, which generate [010] chains of molecules. Adjacent chains in the [001] direction are linked by Cl···π interactions (Riley & Tran, 2017) with C9···*Cg*1($-x$, $-y$, $1-z$) = 3.5088 (12) Å, Cl2···*Cg*1($-x$, $-y$, $1-z$) = 4.005 (3) Å and C9—Cl2···*Cg*1 = 93.77 (9)° where *Cg*1 is the centroid of the thiophene ring. Weak offset face-to-face π–π stacking interactions occur between inversion-related thiophene rings with a centroid–centroid separation *Cg*1···*Cg*1($-x$, $1-y$, $1-z$) of 3.9011 (14) Å. Taken together, the C—H···O, Cl···π and π–π interactions lead to a three-dimensional network.

Synthesis and crystallization

3-Acetyl-2,5-dichlorothiophene was prepared *via* Friedel–Crafts reaction as per the literature procedure (Bachman & Heisey, 1948). The corresponding chalcone, (*E*)-1-(2,5-dichlorothiophen-3-yl)-3-(2,4-dimethoxyphenyl)prop-2-en-1-one, was prepared according to the literature procedure (Al-Refai *et al.*, 2017 and references therein).

(*E*)-1-(2,5-Dichlorothiophen-3-yl)-3-(2,4-dimethoxyphenyl)prop-2-en-1-one (3.0 mmol) and methylhydrazine (4.0 mmol, 1.3 equiv.) were refluxed in 25 ml of ethanol for 5 h until completion of the reaction. The reaction mixture was then cooled, whereupon a solid precipitate was formed. This was filtered off, washed with cold ethanol, and dried. Yellow blocks of **I** were grown by slow evaporation of an ethanol solution. Yield: 89%. ^{1}H NMR (300 MHz, DMSO-d_6, p.p.m.): δ = 7.33 (*d*, *J* = 8.27, 1H, H-6"), 7.27 (*s*, 1H, H-4′), 6.65 (*d*, *J* = 8.44, 1H, H-5"), 6.59 (*s*, 1H, H-3"), 4.39 (*dd*, *J* = 14.06, 10.47, 1H, H-5), 3.80, 3.77 (2*s*, 6H, OCH_3-2",4"), 3.58 (*dd*, *J* = 16.48, 10.38, 1H_A, H-4), 2.76 (*m*, 1H, H_B, H-4), 2.70 (*s*, 3H, N—CH_3).^{13}C NMR (75 MHz, DMSO-d_6, p.p.m.): δ = 159.93, 158.12 (C_q-2",4"), 142.86 (C_q-3), 131.45, 125.40, 121.46, 119.80 (C_q-2′, 3′, 5′, 1"), 127.45, 126.37 (CH-4′, 6″), 105.07 (CH-5″), 98.50 (CH-3″), 66.06 (CH-5), 55.57, 55.19 (OCH_3-2",4"), 41.86 (CH_2-4), 40.88 (NCH_3). **–(+)-ESIMS** *m*/*z* 371 ([*M*+H]$^+$,100), 373 ([*M*+H+2]$^+$,70), 375 ([*M*+H+4]$^+$,15), 393([*M*+Na]$^+$, 20), 395 ([*M*+Na+2]$^+$, 16), 397 ([*M*+Na+4]$^+$, 4). **-(+)-HRESIMS** *m*/*z* 371.0383 [*M*+H]$^+$, 373.0355 [*M*+H+2]$^+$, (calculated for $C_{16}H_{16}Cl_2N_2O_2SH$, 371.0382).

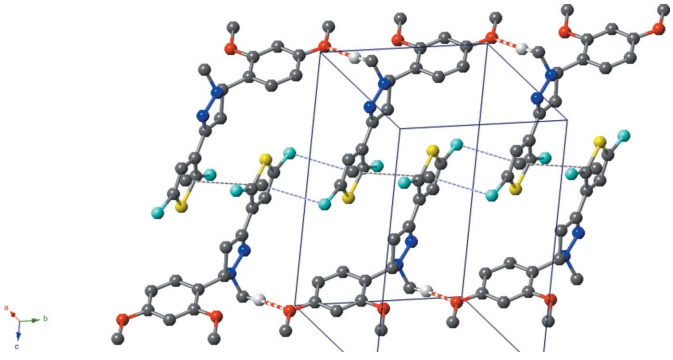


Figure 2
A packing view of **I** showing layers parallel to *bc* plane assembled through C—H···O (rendered multi-band cylinders), Cl···π (gray dashed lines) and π–π (blue dashed lines) interactions. Hydrogen atoms not involved in interactions are omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	1.00	2.39	2.817 (3)	105
C11—H11*C*···O2^{i}	0.98	2.70	3.600 (3)	153
C18—H18*C*···O2^{ii}	0.98	2.68	3.517 (2)	144

Symmetry codes: (i) x, $y-1$, z; (ii) $-x+1$, $-y+2$, $-z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{16}Cl_2N_2O_2S$
M_r	371.27
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.3836 (3), 8.4780 (3), 13.3050 (4)
α, β, γ (°)	97.779 (3), 101.929 (2), 114.967 (2)
V (Å^3)	811.94 (5)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	4.89
Crystal size (mm)	0.17 × 0.14 × 0.12
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Multi-scan (*LANA*; Stoe & Cie, 2016)
T_{min}, T_{max}	0.260, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	21767, 3062, 2794
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.614
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.050, 0.137, 1.05
No. of reflections	3062
No. of parameters	211
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.79, −0.50

Computer programs: *X-AREA* and *LANA* (Stoe & Cie, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*) and *DIAMOND* (Crystal Impact).

Refinement

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

Funding information

The authors thank Al al-Bayt University for financial support. Thanks are also due to the DFG (Deutsche Forschungsgemeinschaft) for financial support (research visit fellowship to Dr Mahmoud Al-Refai).

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full crystallographic data

IUCrData (2019). **4**, x191046 [https://doi.org/10.1107/S2414314619010460]

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Crystal data

$C_{16}H_{16}Cl_2N_2O_2S$
M_r = 371.27
Triclinic, $P\overline{1}$
a = 8.3836 (3) Å
b = 8.4780 (3) Å
c = 13.3050 (4) Å
α = 97.779 (3)°
β = 101.929 (2)°
γ = 114.967 (2)°
V = 811.94 (5) Å^3
Z = 2
$F(000)$ = 384
D_x = 1.519 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 30941 reflections
θ = 3.5–71.7°
μ = 4.89 mm^{-1}
T = 100 K
Block, yellow
0.17 × 0.14 × 0.12 mm

Data collection

Stoe Stadivari diffractometer
Radiation source: GeniX 3D HF Cu
Detector resolution: 5.81 pixels mm^{-1}
rotation method, ω scans
Absorption correction: multi-scan (*LANA*; Stoe & Cie, 2016)
T_{min} = 0.260, T_{max} = 1.000
21767 measured reflections
3062 independent reflections
2794 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 71.3°, θ_{min} = 3.5°
h = −10→8
k = −4→10
l = −16→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.137
S = 1.05
3062 reflections
211 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.117P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 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. The H atoms were included at calculated positions and refined using the riding model with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). Thr CH_3 groups were allowed to rotate about the bond to their next atom to best fit the electron density.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.0524 (2)	0.3616 (2)	0.24617 (13)	0.0167 (4)
O1	0.63312 (18)	0.79340 (19)	0.17276 (12)	0.0201 (3)
Cl1	0.40982 (6)	0.63165 (6)	0.59685 (4)	0.02134 (19)
Cl2	−0.26047 (7)	−0.01538 (6)	0.52260 (4)	0.02362 (19)
O2	0.46909 (19)	1.27080 (19)	0.12925 (12)	0.0202 (3)
N2	0.1173 (2)	0.4670 (2)	0.17701 (13)	0.0161 (4)
C3	0.3126 (3)	0.6004 (3)	0.22968 (15)	0.0150 (4)
H3	0.394688	0.551101	0.210416	0.018*
C4	0.3262 (3)	0.6153 (3)	0.34763 (16)	0.0163 (4)
H4A	0.442394	0.620750	0.388101	0.020*
H4AB	0.315841	0.721586	0.379923	0.020*
C5	0.1609 (3)	0.4417 (3)	0.34130 (16)	0.0153 (4)
C6	0.1101 (3)	0.3698 (3)	0.42980 (16)	0.0157 (4)
C7	0.2065 (3)	0.4389 (3)	0.53541 (16)	0.0164 (4)
S8	0.10142 (7)	0.31227 (6)	0.61630 (4)	0.01945 (19)
C9	−0.0797 (3)	0.1644 (3)	0.50664 (17)	0.0195 (4)
C10	−0.0603 (3)	0.2079 (3)	0.41399 (17)	0.0168 (4)
H10	−0.147743	0.140421	0.346684	0.020*
C11	0.0802 (3)	0.3591 (3)	0.07189 (16)	0.0199 (4)
H11A	0.114750	0.438012	0.024226	0.030*
H11B	−0.051175	0.273750	0.044120	0.030*
H11C	0.152208	0.293102	0.076627	0.030*
C12	0.3582 (3)	0.7768 (3)	0.19820 (15)	0.0150 (4)
C13	0.5195 (3)	0.8720 (3)	0.17247 (15)	0.0155 (4)
C14	0.5623 (3)	1.0375 (3)	0.14841 (15)	0.0165 (4)
H14	0.672513	1.100335	0.130663	0.020*
C15	0.4406 (3)	1.1093 (3)	0.15080 (15)	0.0161 (4)
C16	0.2790 (3)	1.0170 (3)	0.17691 (16)	0.0186 (4)
H16	0.196574	1.066391	0.178851	0.022*
C17	0.2401 (3)	0.8534 (3)	0.19987 (16)	0.0183 (4)
H17	0.129522	0.790838	0.217385	0.022*
C18	0.7935 (3)	0.8799 (3)	0.13908 (17)	0.0194 (4)
H18A	0.855409	0.804449	0.136606	0.029*
H18B	0.877631	0.996621	0.189289	0.029*
H18C	0.757239	0.897638	0.068323	0.029*
C19	0.6361 (3)	1.3732 (3)	0.10549 (18)	0.0213 (4)

H19A	0.641455	1.486915	0.094107	0.032*
H19B	0.639749	1.304878	0.041167	0.032*
H19C	0.741558	1.397937	0.164924	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0173 (8)	0.0128 (8)	0.0178 (9)	0.0038 (7)	0.0070 (7)	0.0052 (7)
O1	0.0160 (7)	0.0155 (7)	0.0316 (8)	0.0061 (6)	0.0122 (6)	0.0105 (6)
Cl1	0.0178 (3)	0.0155 (3)	0.0190 (3)	−0.0003 (2)	0.0012 (2)	0.0018 (2)
Cl2	0.0234 (3)	0.0144 (3)	0.0280 (3)	0.0009 (2)	0.0143 (2)	0.0063 (2)
O2	0.0196 (7)	0.0142 (7)	0.0285 (8)	0.0066 (6)	0.0097 (6)	0.0106 (6)
N2	0.0158 (8)	0.0112 (8)	0.0158 (8)	0.0007 (7)	0.0057 (7)	0.0041 (6)
C3	0.0137 (9)	0.0110 (9)	0.0184 (10)	0.0031 (7)	0.0059 (8)	0.0052 (7)
C4	0.0155 (10)	0.0122 (10)	0.0181 (10)	0.0030 (8)	0.0047 (8)	0.0062 (7)
C5	0.0143 (9)	0.0096 (9)	0.0200 (10)	0.0033 (8)	0.0056 (8)	0.0039 (7)
C6	0.0150 (9)	0.0106 (10)	0.0196 (10)	0.0040 (8)	0.0060 (8)	0.0035 (7)
C7	0.0157 (10)	0.0116 (10)	0.0189 (10)	0.0025 (8)	0.0061 (8)	0.0056 (8)
S8	0.0213 (3)	0.0164 (3)	0.0162 (3)	0.0042 (2)	0.0062 (2)	0.0050 (2)
C9	0.0174 (10)	0.0117 (10)	0.0252 (11)	0.0027 (8)	0.0078 (8)	0.0028 (8)
C10	0.0157 (9)	0.0155 (10)	0.0182 (10)	0.0048 (8)	0.0073 (8)	0.0058 (8)
C11	0.0215 (10)	0.0177 (10)	0.0164 (10)	0.0051 (8)	0.0064 (8)	0.0046 (8)
C12	0.0137 (9)	0.0125 (10)	0.0143 (9)	0.0025 (7)	0.0028 (8)	0.0039 (7)
C13	0.0142 (9)	0.0137 (10)	0.0136 (9)	0.0026 (8)	0.0033 (8)	0.0025 (7)
C14	0.0138 (9)	0.0141 (10)	0.0165 (9)	0.0014 (8)	0.0055 (8)	0.0036 (7)
C15	0.0166 (10)	0.0114 (10)	0.0148 (9)	0.0020 (8)	0.0026 (8)	0.0044 (7)
C16	0.0174 (10)	0.0182 (11)	0.0227 (11)	0.0088 (8)	0.0082 (8)	0.0073 (8)
C17	0.0143 (9)	0.0166 (10)	0.0204 (10)	0.0031 (8)	0.0064 (8)	0.0056 (8)
C18	0.0139 (10)	0.0159 (10)	0.0264 (11)	0.0035 (8)	0.0097 (8)	0.0053 (8)
C19	0.0201 (10)	0.0130 (10)	0.0280 (11)	0.0032 (8)	0.0089 (9)	0.0087 (8)

Geometric parameters (Å, º)

N1—C5	1.289 (3)	C9—C10	1.355 (3)
N1—N2	1.400 (2)	C10—H10	0.9500
O1—C13	1.373 (2)	C11—H11A	0.9800
O1—C18	1.433 (2)	C11—H11B	0.9800
Cl1—C7	1.719 (2)	C11—H11C	0.9800
Cl2—C9	1.713 (2)	C12—C13	1.394 (3)
O2—C15	1.368 (2)	C12—C17	1.397 (3)
O2—C19	1.430 (2)	C13—C14	1.394 (3)
N2—C11	1.457 (3)	C14—C15	1.394 (3)
N2—C3	1.483 (2)	C14—H14	0.9500
C3—C12	1.520 (3)	C15—C16	1.393 (3)
C3—C4	1.534 (3)	C16—C17	1.377 (3)
C3—H3	1.0000	C16—H16	0.9500
C4—C5	1.513 (3)	C17—H17	0.9500
C4—H4A	0.9900	C18—H18A	0.9800

C4—H4AB	0.9900	C18—H18B	0.9800
C5—C6	1.457 (3)	C18—H18C	0.9800
C6—C7	1.371 (3)	C19—H19A	0.9800
C6—C10	1.453 (3)	C19—H19B	0.9800
C7—S8	1.730 (2)	C19—H19C	0.9800
S8—C9	1.728 (2)		

C5—N1—N2	109.43 (16)	N2—C11—H11B	109.5
C13—O1—C18	117.89 (15)	H11A—C11—H11B	109.5
C15—O2—C19	117.63 (15)	N2—C11—H11C	109.5
N1—N2—C11	112.53 (15)	H11A—C11—H11C	109.5
N1—N2—C3	108.77 (15)	H11B—C11—H11C	109.5
C11—N2—C3	115.30 (15)	C13—C12—C17	117.67 (18)
N2—C3—C12	111.22 (15)	C13—C12—C3	122.64 (17)
N2—C3—C4	102.37 (15)	C17—C12—C3	119.61 (17)
C12—C3—C4	113.81 (16)	O1—C13—C12	116.01 (17)
N2—C3—H3	109.7	O1—C13—C14	122.38 (17)
C12—C3—H3	109.7	C12—C13—C14	121.62 (17)
C4—C3—H3	109.7	C13—C14—C15	118.95 (18)
C5—C4—C3	100.78 (16)	C13—C14—H14	120.5
C5—C4—H4A	111.6	C15—C14—H14	120.5
C3—C4—H4A	111.6	O2—C15—C16	115.63 (17)
C5—C4—H4AB	111.6	O2—C15—C14	123.92 (17)
C3—C4—H4AB	111.6	C16—C15—C14	120.44 (18)
H4A—C4—H4AB	109.4	C17—C16—C15	119.31 (18)
N1—C5—C6	119.76 (18)	C17—C16—H16	120.3
N1—C5—C4	113.11 (18)	C15—C16—H16	120.3
C6—C5—C4	126.93 (18)	C16—C17—C12	122.01 (18)
C7—C6—C10	110.74 (18)	C16—C17—H17	119.0
C7—C6—C5	127.51 (18)	C12—C17—H17	119.0
C10—C6—C5	121.75 (18)	O1—C18—H18A	109.5
C6—C7—Cl1	129.46 (16)	O1—C18—H18B	109.5
C6—C7—S8	113.62 (15)	H18A—C18—H18B	109.5
Cl1—C7—S8	116.90 (12)	O1—C18—H18C	109.5
C9—S8—C7	90.03 (10)	H18A—C18—H18C	109.5
C10—C9—Cl2	126.69 (17)	H18B—C18—H18C	109.5
C10—C9—S8	113.60 (16)	O2—C19—H19A	109.5
Cl2—C9—S8	119.71 (13)	O2—C19—H19B	109.5
C9—C10—C6	112.00 (19)	H19A—C19—H19B	109.5
C9—C10—H10	124.0	O2—C19—H19C	109.5
C6—C10—H10	124.0	H19A—C19—H19C	109.5
N2—C11—H11A	109.5	H19B—C19—H19C	109.5

C5—N1—N2—C11	146.57 (17)	S8—C9—C10—C6	0.1 (2)
C5—N1—N2—C3	17.5 (2)	C7—C6—C10—C9	−1.0 (2)
N1—N2—C3—C12	−145.62 (15)	C5—C6—C10—C9	179.62 (17)
C11—N2—C3—C12	86.9 (2)	N2—C3—C12—C13	−136.48 (18)
N1—N2—C3—C4	−23.72 (19)	C4—C3—C12—C13	108.5 (2)

C11—N2—C3—C4	−151.19 (16)	N2—C3—C12—C17	46.9 (2)
N2—C3—C4—C5	20.12 (18)	C4—C3—C12—C17	−68.1 (2)
C12—C3—C4—C5	140.24 (16)	C18—O1—C13—C12	175.41 (17)
N2—N1—C5—C6	172.21 (17)	C18—O1—C13—C14	−4.8 (3)
N2—N1—C5—C4	−3.1 (2)	C17—C12—C13—O1	179.32 (16)
C3—C4—C5—N1	−11.6 (2)	C3—C12—C13—O1	2.7 (3)
C3—C4—C5—C6	173.50 (18)	C17—C12—C13—C14	−0.4 (3)
N1—C5—C6—C7	−178.71 (18)	C3—C12—C13—C14	−177.10 (17)
C4—C5—C6—C7	−4.1 (3)	O1—C13—C14—C15	−179.39 (17)
N1—C5—C6—C10	0.6 (3)	C12—C13—C14—C15	0.3 (3)
C4—C5—C6—C10	175.16 (16)	C19—O2—C15—C16	177.97 (18)
C10—C6—C7—Cl1	−177.09 (14)	C19—O2—C15—C14	−1.6 (3)
C5—C6—C7—Cl1	2.3 (3)	C13—C14—C15—O2	179.59 (17)
C10—C6—C7—S8	1.5 (2)	C13—C14—C15—C16	0.0 (3)
C5—C6—C7—S8	−179.20 (16)	O2—C15—C16—C17	−179.91 (18)
C6—C7—S8—C9	−1.20 (16)	C14—C15—C16—C17	−0.3 (3)
Cl1—C7—S8—C9	177.54 (12)	C15—C16—C17—C12	0.2 (3)
C7—S8—C9—C10	0.60 (17)	C13—C12—C17—C16	0.2 (3)
C7—S8—C9—Cl2	−179.08 (13)	C3—C12—C17—C16	176.92 (18)
Cl2—C9—C10—C6	179.76 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1	1.00	2.39	2.817 (3)	105
C11—H11*C*···O2^{i}	0.98	2.70	3.600 (3)	153
C18—H18*C*···O2^{ii}	0.98	2.68	3.517 (2)	144

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