Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Methyl-3-trifluoromethyl-5-[(3-chlorophenyl)sulfanyl]-1*H*-pyrazole-4-carbaldehyde *O*-(4-chlorobenzoyl)oxime

Hong Dai, Hai-Jun Zhang, Lei Shi, Kun-Peng Luo and Yu-Jun Shi*

College of Chemistry and Chemical Engineering, Nantong University, Nantong 226019, Peoples' Republic of China
Correspondence e-mail: nankaidx228@yahoo.com.cn

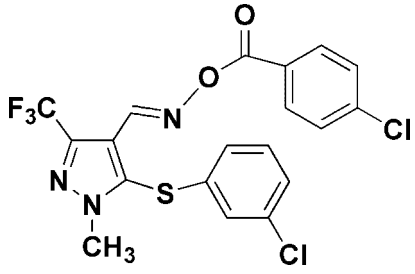
Received 4 November 2011; accepted 11 November 2011

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.049; wR factor = 0.137; data-to-parameter ratio = 13.4.

In the title compound, $C_{19}H_{12}Cl_2F_3N_3O_2S$, the 3-chlorophenyl and 4-chlorophenyl rings form dihedral angles 89.5 (2) and 11.4 (2)°, respectively, with the pyrazole ring. In the crystal, molecules related by translation along the *a* axis are linked into chains *via* C—H···N hydrogen bonds.

Related literature

For the crystal structure of a related pyrazole oxime studied recently by our group, see: Dai *et al.* (2011).



Experimental

Crystal data

$C_{19}H_{12}Cl_2F_3N_3O_2S$
M_r = 474.28
Monoclinic, $P2_1/n$
a = 8.1405 (16) Å
b = 18.680 (4) Å
c = 13.737 (3) Å
β = 96.10 (3)°
V = 2077.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 113 K
0.18 × 0.16 × 0.12 mm

Data collection

Rigaku Saturn CCD area detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)
T_{min} = 0.922, T_{max} = 0.947
11802 measured reflections
3654 independent reflections
2794 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.137
S = 1.10
3654 reflections
273 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 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}	0.93	2.49	3.365 (4)	156

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

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

This work was supported by the National Natural Science Foundation of China (NNSFC) (grant No. 20772068), the Science and Technology Projects Fund of Nantong City (grant Nos. K2010016 and AS2010005), the Science Foundation of Nantong University (grant Nos. 09Z010 and 09C001) and the Scientific Research Foundation for Talent Introduction of Nantong University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5193).

References

Dai, H., Shen, Y.-F., Chen, J., Chen, H.-L. & Shen, Y.-J. (2011). *Acta Cryst.* E**67**, o726.
Rigaku (2008). *CrystalClear*. Rigaku Corporation, Toyko, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2011). E**67**, o3343 [**doi:10.1107/S1600536811047970**]

1-Methyl-3-trifluoromethyl-5-[(3-chlorophenyl)sulfanyl]-1*H*-pyrazole-4-carbaldehyde *O*-(4-chlorobenzoyl)oxime

H. Dai, H.-J. Zhang, L. Shi, K.-P. Luo and Y.-J. Shi

Comment

As a continuation of our structural investigation of pyrazole oxime esters (Dai *et al.*, 2011), we report here the structure of the title compound (I).

In (I) (Fig. 1), all bonds lengths and angles are comparable with those observed in the related compound (Dai *et al.*, 2011). The mean planes p1 (C7/C8/C9/N2/N1), p2 (C1/C2/C3/C4/C5/C6) and p3 (C13/C14/C15/C16/C17/C18) form the following dihedral angles - p2/p1 89.5 (2)°, p3/p1 11.4 (3)°. The crystal packing shows weak intermolecular C—H···N interactions (Table 1), which link molecules into chains along the *a* axis.

Experimental

To a well stirred solution of 1-methyl-3-trifluoromethyl-5-(3-chlorophenthio)- 1*H*-pyrazole-4-carbaldehyde oxime (4 mmol), and pyridine (5 ml) in 40 ml of dichloromethane, was added dropwise 4-chlorobenzoyl chloride (5 mmol) at room temperature. The resulting solution was heated to reflux for 7 h and cooled to room temperature. The mixture was washed with saturated brine (3 * 30 ml) and dried over anhydrous sodium sulfate. The solvent was evaporated under reduced pressure, the residue was separated by column chromatography on silica gel with petroleum ether/ethyl acetate (12:1 *v*/*v*) as eluent, and then recrystallized from petroleum ether/ethyl acetate acetate to give a colourless crystal.

Refinement

All H atoms were placed in calculated positions, with C–H = 0.93 - 0.96 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2-1.5 U_{eq}(C).

Figures

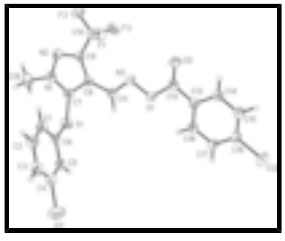


Fig. 1. The molecular structure of (I) showing the atomic numbering and 30% probabilty displacement ellipsoids.

1-Methyl-3-trifluoromethyl-5-[(3-chlorophenyl)sulfanyl]-1*H*-pyrazole-4- carbaldehyde *O*-(4-chlorobenzoyl)oxime

Crystal data

$C_{19}H_{12}Cl_2F_3N_3O_2S$	$F(000) = 960$
$M_r = 474.28$	$D_x = 1.517$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 4368 reflections
$a = 8.1405$ (16) Å	$\theta = 2.2$–$27.9°$
$b = 18.680$ (4) Å	$\mu = 0.46$ mm^{-1}
$c = 13.737$ (3) Å	$T = 113$ K
$\beta = 96.10$ (3)°	Monoclinic, colourless
$V = 2077.0$ (7) Å^3	0.18 × 0.16 × 0.12 mm
$Z = 4$	

Data collection

Rigaku Saturn CCD area detector diffractometer	3654 independent reflections
Radiation source: rotating anode	2794 reflections with $I > 2\sigma(I)$
confocal	$R_{int} = 0.039$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
ω and φ scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2008)	$k = -22 \rightarrow 22$
$T_{min} = 0.922$, $T_{max} = 0.947$	$l = -14 \rightarrow 16$
11802 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.137$	$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2 + 0.2323P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.10$	$(\Delta/\sigma)_{max} = 0.001$
3654 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
273 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.020 (3)

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 $F^2 > \sigma(F^2)$ 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}
Cl1	1.09484 (13)	0.84104 (6)	0.56388 (10)	0.1131 (4)
Cl2	1.29709 (11)	0.74602 (6)	1.34884 (7)	0.0961 (4)
S1	0.64859 (10)	1.00969 (4)	0.71200 (6)	0.0663 (3)
F1	0.1729 (2)	0.85215 (8)	0.92153 (14)	0.0775 (5)
F2	−0.0064 (2)	0.93357 (11)	0.88380 (14)	0.0867 (6)
F3	0.1826 (2)	0.94978 (10)	1.00144 (12)	0.0778 (5)
O1	0.6832 (2)	0.87708 (10)	1.04766 (12)	0.0532 (5)
O2	0.5304 (3)	0.84250 (12)	1.16752 (17)	0.0833 (7)
N1	0.3126 (3)	1.00802 (11)	0.71276 (16)	0.0566 (6)
N2	0.1875 (3)	0.98695 (11)	0.76284 (16)	0.0543 (6)
N3	0.5309 (3)	0.89838 (12)	0.99338 (15)	0.0538 (6)
C1	0.5668 (4)	0.88041 (15)	0.6144 (2)	0.0607 (7)
H1	0.4569	0.8886	0.6238	0.073*
C2	0.6110 (4)	0.81988 (17)	0.5655 (2)	0.0688 (8)
H2	0.5297	0.7873	0.5423	0.083*
C3	0.7709 (4)	0.80690 (17)	0.5504 (2)	0.0715 (8)
H3	0.7993	0.7657	0.5180	0.086*
C4	0.8894 (4)	0.85576 (16)	0.5841 (2)	0.0654 (8)
C5	0.8510 (3)	0.91618 (15)	0.63472 (18)	0.0584 (7)
H5	0.9336	0.9479	0.6587	0.070*
C6	0.6885 (3)	0.92892 (14)	0.64942 (16)	0.0508 (6)
C7	0.4631 (3)	0.98935 (13)	0.75808 (18)	0.0492 (6)
C8	0.4342 (3)	0.95423 (12)	0.84390 (16)	0.0434 (6)
C9	0.2602 (3)	0.95408 (12)	0.84192 (16)	0.0433 (6)
C10	0.1528 (3)	0.92283 (13)	0.91187 (19)	0.0518 (6)
C11	0.5643 (3)	0.92724 (12)	0.91488 (18)	0.0468 (6)
H11	0.6739	0.9313	0.9023	0.056*
C12	0.6607 (3)	0.84774 (13)	1.13649 (19)	0.0513 (6)
C13	0.8222 (3)	0.82499 (13)	1.18756 (18)	0.0473 (6)
C14	0.8200 (4)	0.77728 (14)	1.2655 (2)	0.0584 (7)
H14	0.7197	0.7611	1.2838	0.070*
C15	0.9663 (4)	0.75393 (14)	1.3154 (2)	0.0629 (8)
H15	0.9651	0.7220	1.3673	0.076*

C16	1.1137 (3)	0.77827 (15)	1.2879 (2)	0.0582 (7)
C17	1.1198 (3)	0.82612 (14)	1.2119 (2)	0.0555 (7)
H17	1.2206	0.8425	1.1946	0.067*
C18	0.9727 (3)	0.84924 (13)	1.16177 (19)	0.0517 (6)
H18	0.9749	0.8814	1.1102	0.062*
C19	0.2742 (5)	1.0461 (2)	0.6195 (2)	0.0884 (11)
H19A	0.2762	1.0130	0.5662	0.133*
H19B	0.3549	1.0830	0.6139	0.133*
H19C	0.1665	1.0673	0.6176	0.133*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0650 (6)	0.1302 (9)	0.1451 (10)	0.0138 (5)	0.0163 (6)	−0.0332 (7)
Cl2	0.0651 (6)	0.1262 (8)	0.0921 (6)	0.0249 (5)	−0.0154 (5)	0.0214 (5)
S1	0.0663 (5)	0.0631 (5)	0.0734 (5)	−0.0207 (3)	0.0257 (4)	−0.0077 (3)
F1	0.0803 (13)	0.0574 (10)	0.0992 (13)	−0.0039 (8)	0.0302 (10)	0.0083 (8)
F2	0.0379 (9)	0.1262 (16)	0.0967 (13)	0.0030 (9)	0.0103 (9)	0.0184 (11)
F3	0.0809 (13)	0.0988 (13)	0.0579 (10)	−0.0146 (10)	0.0263 (9)	−0.0142 (9)
O1	0.0370 (10)	0.0717 (11)	0.0500 (9)	0.0044 (8)	0.0002 (8)	0.0088 (8)
O2	0.0458 (13)	0.1175 (18)	0.0892 (15)	0.0122 (11)	0.0195 (12)	0.0396 (13)
N1	0.0603 (15)	0.0591 (13)	0.0498 (12)	0.0021 (11)	0.0025 (11)	0.0099 (10)
N2	0.0485 (13)	0.0582 (12)	0.0553 (13)	0.0069 (10)	0.0016 (11)	0.0036 (10)
N3	0.0374 (12)	0.0684 (14)	0.0536 (12)	0.0051 (10)	−0.0040 (10)	0.0042 (10)
C1	0.0530 (17)	0.0707 (17)	0.0595 (16)	−0.0153 (13)	0.0109 (13)	−0.0025 (13)
C2	0.072 (2)	0.0704 (18)	0.0629 (17)	−0.0216 (16)	0.0033 (16)	−0.0037 (14)
C3	0.080 (2)	0.0724 (19)	0.0627 (18)	−0.0051 (17)	0.0113 (16)	−0.0053 (15)
C4	0.0582 (19)	0.079 (2)	0.0587 (16)	0.0060 (15)	0.0049 (14)	0.0002 (14)
C5	0.0490 (17)	0.0761 (18)	0.0486 (14)	−0.0088 (13)	−0.0013 (12)	0.0014 (13)
C6	0.0522 (16)	0.0591 (15)	0.0413 (13)	−0.0098 (12)	0.0052 (12)	0.0070 (11)
C7	0.0483 (16)	0.0499 (13)	0.0498 (14)	−0.0037 (11)	0.0070 (12)	0.0012 (11)
C8	0.0411 (14)	0.0457 (12)	0.0432 (12)	−0.0016 (10)	0.0038 (10)	−0.0044 (10)
C9	0.0401 (14)	0.0469 (12)	0.0424 (12)	0.0035 (10)	0.0017 (10)	−0.0022 (10)
C10	0.0383 (15)	0.0564 (15)	0.0611 (16)	0.0019 (11)	0.0067 (12)	−0.0012 (12)
C11	0.0360 (13)	0.0532 (14)	0.0509 (14)	−0.0006 (10)	0.0026 (11)	−0.0028 (11)
C12	0.0453 (16)	0.0537 (14)	0.0549 (15)	−0.0002 (11)	0.0050 (13)	0.0065 (11)
C13	0.0425 (15)	0.0488 (13)	0.0505 (13)	0.0023 (11)	0.0048 (11)	0.0007 (11)
C14	0.0511 (16)	0.0626 (16)	0.0623 (16)	0.0010 (13)	0.0105 (13)	0.0150 (13)
C15	0.062 (2)	0.0667 (17)	0.0598 (17)	0.0091 (14)	0.0049 (14)	0.0170 (13)
C16	0.0517 (17)	0.0651 (16)	0.0554 (15)	0.0111 (13)	−0.0057 (13)	0.0009 (13)
C17	0.0418 (15)	0.0617 (16)	0.0627 (16)	−0.0018 (12)	0.0036 (13)	−0.0007 (13)
C18	0.0469 (16)	0.0531 (14)	0.0547 (14)	−0.0015 (11)	0.0032 (12)	0.0072 (11)
C19	0.103 (3)	0.096 (2)	0.0642 (19)	0.011 (2)	0.0001 (18)	0.0349 (18)

Geometric parameters (Å, °)

Cl1—C4	1.746 (3)	C4—C5	1.379 (4)
Cl2—C16	1.740 (3)	C5—C6	1.380 (4)
S1—C7	1.740 (3)	C5—H5	0.9300

S1—C6	1.783 (3)	C7—C8	1.391 (3)
F1—C10	1.335 (3)	C8—C9	1.414 (3)
F2—C10	1.327 (3)	C8—C11	1.451 (3)
F3—C10	1.328 (3)	C9—C10	1.486 (4)
O1—C12	1.368 (3)	C11—H11	0.9300
O1—N3	1.434 (2)	C12—C13	1.485 (3)
O2—C12	1.189 (3)	C13—C18	1.387 (4)
N1—N2	1.347 (3)	C13—C14	1.394 (4)
N1—C7	1.359 (3)	C14—C15	1.381 (4)
N1—C19	1.469 (3)	C14—H14	0.9300
N2—C9	1.331 (3)	C15—C16	1.373 (4)
N3—C11	1.261 (3)	C15—H15	0.9300
C1—C2	1.382 (4)	C16—C17	1.380 (4)
C1—C6	1.390 (4)	C17—C18	1.385 (4)
C1—H1	0.9300	C17—H17	0.9300
C2—C3	1.361 (4)	C18—H18	0.9300
C2—H2	0.9300	C19—H19A	0.9600
C3—C4	1.372 (4)	C19—H19B	0.9600
C3—H3	0.9300	C19—H19C	0.9600
C7—S1—C6	101.54 (12)	F2—C10—F1	106.5 (2)
C12—O1—N3	112.63 (19)	F3—C10—F1	105.9 (2)
N2—N1—C7	112.6 (2)	F2—C10—C9	112.1 (2)
N2—N1—C19	119.0 (3)	F3—C10—C9	112.8 (2)
C7—N1—C19	128.4 (3)	F1—C10—C9	112.2 (2)
C9—N2—N1	104.9 (2)	N3—C11—C8	121.0 (2)
C11—N3—O1	108.1 (2)	N3—C11—H11	119.5
C2—C1—C6	119.3 (3)	C8—C11—H11	119.5
C2—C1—H1	120.4	O2—C12—O1	124.2 (2)
C6—C1—H1	120.4	O2—C12—C13	125.9 (2)
C3—C2—C1	121.5 (3)	O1—C12—C13	109.9 (2)
C3—C2—H2	119.3	C18—C13—C14	119.2 (2)
C1—C2—H2	119.3	C18—C13—C12	123.2 (2)
C2—C3—C4	118.7 (3)	C14—C13—C12	117.6 (2)
C2—C3—H3	120.7	C15—C14—C13	120.2 (3)
C4—C3—H3	120.7	C15—C14—H14	119.9
C3—C4—C5	121.7 (3)	C13—C14—H14	119.9
C3—C4—Cl1	119.5 (3)	C16—C15—C14	119.4 (3)
C5—C4—Cl1	118.8 (2)	C16—C15—H15	120.3
C4—C5—C6	119.1 (3)	C14—C15—H15	120.3
C4—C5—H5	120.4	C15—C16—C17	121.7 (2)
C6—C5—H5	120.4	C15—C16—Cl2	118.9 (2)
C5—C6—C1	119.7 (3)	C17—C16—Cl2	119.4 (2)
C5—C6—S1	116.3 (2)	C16—C17—C18	118.6 (3)
C1—C6—S1	124.0 (2)	C16—C17—H17	120.7
N1—C7—C8	106.5 (2)	C18—C17—H17	120.7
N1—C7—S1	123.51 (19)	C17—C18—C13	120.8 (2)
C8—C7—S1	130.0 (2)	C17—C18—H18	119.6
C7—C8—C9	104.1 (2)	C13—C18—H18	119.6
C7—C8—C11	123.8 (2)	N1—C19—H19A	109.5

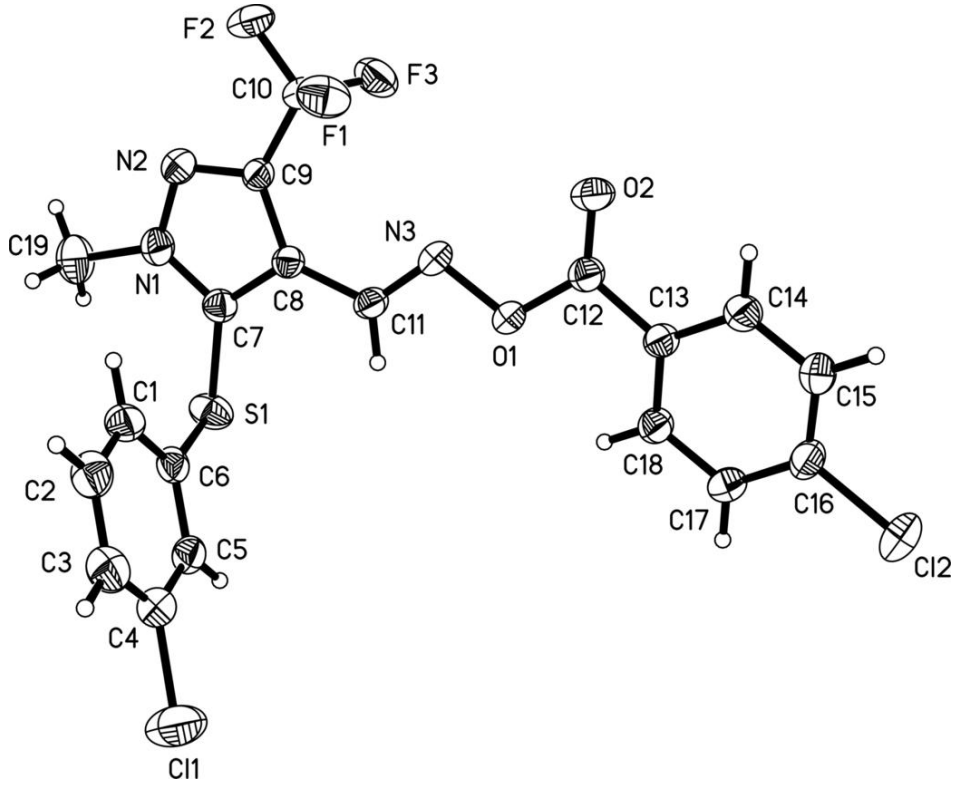
C9—C8—C11	132.1 (2)	N1—C19—H19B	109.5
N2—C9—C8	111.9 (2)	H19A—C19—H19B	109.5
N2—C9—C10	117.9 (2)	N1—C19—H19C	109.5
C8—C9—C10	130.2 (2)	H19A—C19—H19C	109.5
F2—C10—F3	106.8 (2)	H19B—C19—H19C	109.5
C7—N1—N2—C9	0.0 (3)	C11—C8—C9—N2	178.2 (2)
C19—N1—N2—C9	179.5 (2)	C7—C8—C9—C10	178.2 (2)
C12—O1—N3—C11	177.4 (2)	C11—C8—C9—C10	−2.8 (4)
C6—C1—C2—C3	−0.3 (4)	N2—C9—C10—F2	−0.6 (3)
C1—C2—C3—C4	−0.7 (5)	C8—C9—C10—F2	−179.5 (2)
C2—C3—C4—C5	1.8 (5)	N2—C9—C10—F3	−121.2 (2)
C2—C3—C4—Cl1	−179.0 (2)	C8—C9—C10—F3	59.9 (3)
C3—C4—C5—C6	−2.0 (4)	N2—C9—C10—F1	119.2 (2)
Cl1—C4—C5—C6	178.8 (2)	C8—C9—C10—F1	−59.7 (3)
C4—C5—C6—C1	0.9 (4)	O1—N3—C11—C8	179.75 (19)
C4—C5—C6—S1	−178.0 (2)	C7—C8—C11—N3	177.1 (2)
C2—C1—C6—C5	0.2 (4)	C9—C8—C11—N3	−1.7 (4)
C2—C1—C6—S1	179.0 (2)	N3—O1—C12—O2	−2.5 (4)
C7—S1—C6—C5	−157.1 (2)	N3—O1—C12—C13	178.37 (19)
C7—S1—C6—C1	24.0 (2)	O2—C12—C13—C18	−161.7 (3)
N2—N1—C7—C8	−0.5 (3)	O1—C12—C13—C18	17.4 (3)
C19—N1—C7—C8	−179.9 (3)	O2—C12—C13—C14	17.8 (4)
N2—N1—C7—S1	−179.46 (17)	O1—C12—C13—C14	−163.0 (2)
C19—N1—C7—S1	1.1 (4)	C18—C13—C14—C15	−0.8 (4)
C6—S1—C7—N1	−96.1 (2)	C12—C13—C14—C15	179.7 (3)
C6—S1—C7—C8	85.2 (2)	C13—C14—C15—C16	0.2 (4)
N1—C7—C8—C9	0.7 (2)	C14—C15—C16—C17	0.5 (4)
S1—C7—C8—C9	179.61 (19)	C14—C15—C16—Cl2	−177.8 (2)
N1—C7—C8—C11	−178.3 (2)	C15—C16—C17—C18	−0.7 (4)
S1—C7—C8—C11	0.6 (4)	Cl2—C16—C17—C18	177.6 (2)
N1—N2—C9—C8	0.5 (3)	C16—C17—C18—C13	0.2 (4)
N1—N2—C9—C10	−178.6 (2)	C14—C13—C18—C17	0.6 (4)
C7—C8—C9—N2	−0.8 (3)	C12—C13—C18—C17	−179.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···N2^{i}	0.93	2.49	3.365 (4)	156

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

Fig. 1


F2
C10
F3
F1
N2
C9
O2
N3
C19
N1
C8
C11
O1
C12
C13
C14
C7
C15
C1
S1
C18
C6
C2
C16
C17
C5
C3
Cl2
C4
Cl1