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2-(4,6-Dimethoxypyrimidine-2-ylsulfanyl)-*N*-(3-nitrophenyl)benzamide

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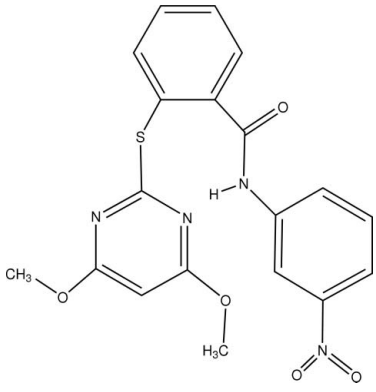
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 13.9.

The title compound, $C_{19}H_{16}N_4O_5S$, was synthesized by the reaction of 2-(4,6-dimethoxypyrimidine-2-ylsulfanyl)benzoic acid and 3-nitroaniline in the presence of *N*,*N*′-dicyclohexylcarbodiimide catalyst in dichloromethane. Intramolecular N—H···N hydrogen bonds are found in the crystal structure.

Related literature

For related literature, see: Hall *et al.* (1999); Hudson *et al.* (2002); Lin *et al.* (2001); Nezu *et al.* (1996); Park *et al.* (2005); Tamaru *et al.* (1997).



Experimental

Crystal data

$C_{19}H_{16}N_4O_5S$
M_r = 412.42
Monoclinic, *Cc*
a = 18.3554 (9) Å
b = 12.3477 (6) Å
c = 8.4209 (5) Å
β = 91.0467 (17)°
V = 1908.25 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 (1) K
0.46 × 0.42 × 0.38 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.904, T_{max} = 0.923
8657 measured reflections
3670 independent reflections
3417 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.02
3670 reflections
264 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), 1523 Friedel pairs
Flack parameter: 0.10 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H111···N3	0.86	2.10	2.914 (2)	158

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2230).

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supplementary materials

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2-(4,6-Dimethoxypyrimidine-2-ylsulfanyl)-*N*-(3-nitrophenyl)benzamide

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Comment

4,6-Dimethoxypyrimidines with a phenoxy substructure at the 2-position exhibit marked herbicidal activity (Nezu *et al.*, 1996; Tamaru *et al.*, 1997; Hudson *et al.*, 2002). The title compound, (I,) has showed herbicidal activity against various grass and broadleaf weeds. The present X-ray crystal structure analysis was undertaken for understanding the relationship between structure and activity.

The bond lengths and angles in the pyrimidine moiety are close to those found in related compounds (Hall *et al.*, 1999; Lin *et al.*, 2001). Particularly, the angle N3—C14—N4 [125.68 (1)°] deviates significantly from the normal value. In the two benzene rings, the angles are close to 120° which are close to $C_{aromatic}$—$C_{aromatic}$—C = 120° (Park *et al.*, 2005). There is an N—H.·N intramolecular hydrogen bond between the proton on N1 and the pyrimidine nitrogen N3. Weak C—H···O, C—H···S and C—H···π interactions give rise to the formation of a 3-D network.

Experimental

N,*N*'-dicyclohexylcarbodiimide (1.08 g,0.055 mol) dissolved in 10 ml of dichloromethane was added dropwise over 20 minutes to the vortex of a stirred solution of 2-(4,6-dimethoxypyrimidin-2-ylsulfanyl)benzoic acid (1.60 g,0.0055 mol) and 3-nitrobenzenamine (0.69 g,0.005 mol) in 30 ml dichloromethane at 273 K. Subsequently,the mixture was stirred 6 h more at room temperature and the resulting solution filtered and washed with dichloromethane. A solution of 50 ml of 10% sodium hydroxide was added and stirred 1 h more and extracted twice with dichloromethane. The separated dichloromethane layer, dried with magnesium sulfate, was evaporated *in vacuo* leaving a crude of white powder. These crystals were dissolved in ethanol and left to slowly evaporate at room temperature. After 5 d, single crystals suitable for X-ray analysis were obtained (m.p. 399–402 K).

Refinement

All H atoms were placed in calculated positions with C—H = 0.93Å (aromatic) or C—H=0.96Å (methoxy) and N—H = 0.86 Å, and included in the final cycles of refinement in the riding-model approximation,with U_{iso}(H) = 1.2U_{eq} of the carrier atoms.

Figures

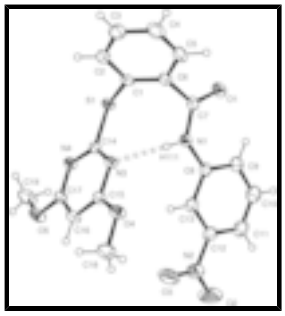


Fig. 1. The molecular structure of (I), showing the hydrogen bond N1—H111—N3, with displacement ellipsoids drawn at the 50% probability level.

2-(4,6-Dimethoxypyrimidine-2-ylsulfanyl)-*N*-(3-nitrophenyl)benzamide

Crystal data

$C_{19}H_{16}N_4O_5S$	F_{000} = 856.00
M_r = 412.42	D_x = 1.435 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: C -2yc	Cell parameters from 10239 reflections
a = 18.3554 (9) Å	θ = 3.1–27.4º
b = 12.3477 (6) Å	μ = 0.21 mm^{-1}
c = 8.4209 (5) Å	*T* = 298 (1) K
β = 91.0467 (17)º	Chunk, colorless
V = 1908.25 (17) Å^3	0.46 × 0.42 × 0.38 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3417 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.022
ω scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −21→23
T_{min} = 0.904, T_{max} = 0.923	*k* = −15→15
8657 measured reflections	*l* = −10→10
3670 independent reflections	

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max}$ < 0.001
$R[F^2 > 2\sigma(F^2)]$ = 0.032	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$wR(F^2)$ = 0.081	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
S = 1.02	Extinction correction: Larson (1970)
3670 reflections	Extinction coefficient: 105 (15)

264 parameters
H-atom parameters constrained
$w = 1/[0.0009F_o^2 + 1.0000\sigma(F_o^2)]/(4F_o^2)$

Absolute structure: Flack (1983), 1523 Friedel pairs
Flack parameter: 0.10 (5)

Special details

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (S) are based on F^2. *R*-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.38203 (3)	0.89646 (3)	1.00620 (6)	0.03648 (10)
O1	0.20595 (9)	0.69864 (12)	0.8983 (2)	0.0557 (4)
O2	0.50881 (17)	0.37440 (19)	0.5022 (4)	0.1185 (10)
O3	0.52021 (13)	0.54516 (18)	0.4747 (3)	0.1079 (9)
O4	0.46729 (6)	0.83461 (12)	0.45837 (14)	0.0450 (3)
O5	0.64111 (8)	0.86050 (14)	0.86357 (17)	0.0523 (4)
N1	0.31393 (9)	0.71447 (12)	0.76172 (19)	0.0401 (4)
N2	0.48791 (12)	0.46688 (18)	0.5254 (2)	0.0716 (7)
N3	0.43379 (8)	0.86439 (12)	0.71021 (16)	0.0323 (3)
N4	0.51846 (9)	0.88144 (12)	0.92085 (18)	0.0355 (3)
C1	0.30560 (10)	0.94420 (14)	0.8979 (2)	0.0354 (4)
C2	0.29690 (11)	1.05629 (16)	0.8877 (2)	0.0471 (5)
C3	0.23477 (13)	1.09949 (17)	0.8202 (3)	0.0588 (6)
C4	0.18135 (12)	1.0331 (2)	0.7665 (3)	0.0617 (7)
C5	0.18849 (12)	0.92221 (19)	0.7784 (2)	0.0528 (5)
C6	0.25096 (10)	0.87629 (13)	0.8422 (2)	0.0382 (4)
C7	0.25500 (10)	0.75374 (14)	0.8420 (2)	0.0393 (4)
C8	0.33403 (10)	0.60581 (13)	0.7330 (2)	0.0387 (4)
C9	0.29172 (12)	0.51721 (16)	0.7826 (2)	0.0528 (6)
C10	0.31533 (16)	0.41336 (18)	0.7446 (3)	0.0676 (7)
C11	0.37916 (14)	0.39460 (17)	0.6621 (3)	0.0619 (7)
C12	0.41987 (12)	0.48333 (16)	0.6158 (2)	0.0495 (5)
C13	0.39828 (12)	0.58838 (14)	0.6484 (2)	0.0454 (5)
C14	0.45121 (9)	0.88014 (12)	0.8598 (2)	0.0299 (3)
C15	0.48988 (10)	0.85016 (13)	0.60663 (19)	0.0330 (4)
C16	0.56137 (10)	0.84840 (14)	0.6536 (2)	0.0382 (4)
C17	0.57184 (10)	0.86377 (13)	0.8152 (2)	0.0357 (4)
C18	0.52246 (12)	0.8213 (2)	0.3362 (2)	0.0561 (6)
C19	0.65252 (12)	0.8676 (2)	1.0318 (2)	0.0663 (7)
H2	0.3333	1.1019	0.9269	0.057*
H3	0.2295	1.1742	0.8114	0.071*
H4	0.1392	1.0625	0.7210	0.074*
H5	0.1507	0.8778	0.7429	0.063*
H9	0.2492	0.5278	0.8390	0.063*
H10	0.2875	0.3544	0.7756	0.081*
H11	0.3941	0.3245	0.6386	0.074*

H13	0.4260	0.6468	0.6147	0.055*
H16	0.5994	0.8379	0.5838	0.046*
H111	0.3426	0.7627	0.7237	0.048*
H181	0.5529	0.8845	0.3338	0.067*
H182	0.5518	0.7589	0.3603	0.067*
H183	0.4988	0.8119	0.2345	0.067*
H191	0.6268	0.8100	1.0829	0.080*
H192	0.6348	0.9360	1.0691	0.080*
H193	0.7036	0.8616	1.0564	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0305 (2)	0.0476 (2)	0.03144 (19)	0.0019 (2)	0.00422 (12)	−0.00328 (18)
O1	0.0418 (8)	0.0508 (7)	0.0751 (10)	−0.0089 (7)	0.0182 (7)	0.0001 (6)
O2	0.112 (2)	0.0647 (11)	0.181 (2)	0.0312 (13)	0.0587 (19)	−0.0176 (14)
O3	0.0800 (16)	0.0715 (12)	0.174 (2)	0.0058 (12)	0.0649 (16)	−0.0083 (13)
O4	0.0333 (7)	0.0721 (8)	0.0296 (5)	0.0036 (6)	0.0002 (5)	−0.0037 (5)
O5	0.0267 (6)	0.0909 (10)	0.0390 (7)	0.0035 (6)	−0.0050 (5)	−0.0005 (6)
N1	0.0320 (8)	0.0336 (7)	0.0547 (9)	−0.0044 (6)	0.0059 (6)	−0.0015 (5)
N2	0.0611 (14)	0.0560 (12)	0.0982 (16)	0.0114 (10)	0.0141 (11)	−0.0125 (10)
N3	0.0250 (7)	0.0396 (6)	0.0324 (7)	−0.0014 (5)	0.0012 (5)	0.0010 (5)
N4	0.0283 (7)	0.0449 (7)	0.0333 (7)	0.0014 (6)	−0.0004 (5)	−0.0003 (5)
C1	0.0255 (8)	0.0412 (8)	0.0397 (9)	0.0036 (7)	0.0071 (6)	−0.0028 (6)
C2	0.0387 (11)	0.0394 (9)	0.0633 (12)	−0.0017 (8)	0.0074 (8)	−0.0041 (8)
C3	0.0489 (13)	0.0406 (10)	0.0871 (17)	0.0083 (9)	0.0076 (11)	0.0062 (10)
C4	0.0385 (12)	0.0606 (12)	0.0859 (16)	0.0141 (10)	−0.0037 (11)	0.0098 (11)
C5	0.0284 (10)	0.0566 (10)	0.0732 (13)	0.0002 (9)	−0.0038 (8)	0.0000 (9)
C6	0.0287 (9)	0.0410 (8)	0.0449 (9)	0.0014 (7)	0.0041 (7)	−0.0006 (7)
C7	0.0306 (9)	0.0431 (8)	0.0440 (9)	−0.0051 (7)	−0.0004 (6)	−0.0024 (7)
C8	0.0365 (10)	0.0346 (8)	0.0446 (9)	−0.0032 (7)	−0.0074 (7)	−0.0017 (6)
C9	0.0487 (13)	0.0421 (10)	0.0677 (13)	−0.0087 (9)	0.0082 (9)	0.0006 (8)
C10	0.0665 (17)	0.0381 (10)	0.099 (2)	−0.0090 (11)	0.0114 (13)	0.0031 (10)
C11	0.0656 (16)	0.0355 (9)	0.0845 (17)	0.0023 (10)	−0.0022 (12)	−0.0056 (9)
C12	0.0466 (12)	0.0445 (10)	0.0572 (11)	0.0050 (9)	−0.0029 (9)	−0.0079 (8)
C13	0.0419 (11)	0.0378 (8)	0.0565 (11)	−0.0013 (8)	−0.0001 (8)	−0.0040 (7)
C14	0.0252 (8)	0.0314 (7)	0.0332 (7)	−0.0005 (6)	0.0022 (5)	0.0015 (5)
C15	0.0302 (8)	0.0388 (8)	0.0299 (8)	0.0009 (7)	0.0008 (6)	0.0032 (6)
C16	0.0286 (8)	0.0517 (9)	0.0344 (8)	0.0019 (7)	0.0048 (6)	0.0030 (7)
C17	0.0244 (8)	0.0441 (8)	0.0386 (8)	0.0006 (7)	−0.0011 (6)	0.0035 (7)
C18	0.0487 (12)	0.0900 (15)	0.0297 (9)	0.0020 (11)	0.0061 (8)	−0.0040 (9)
C19	0.0338 (12)	0.121 (2)	0.0436 (11)	0.0063 (12)	−0.0112 (8)	−0.0028 (12)

Geometric parameters (Å, °)

S1—C1	1.7608 (18)	C8—C13	1.405 (2)
S1—C14	1.7973 (17)	C9—C10	1.393 (3)
O1—C7	1.231 (2)	C10—C11	1.393 (4)
O2—N2	1.221 (3)	C11—C12	1.386 (3)

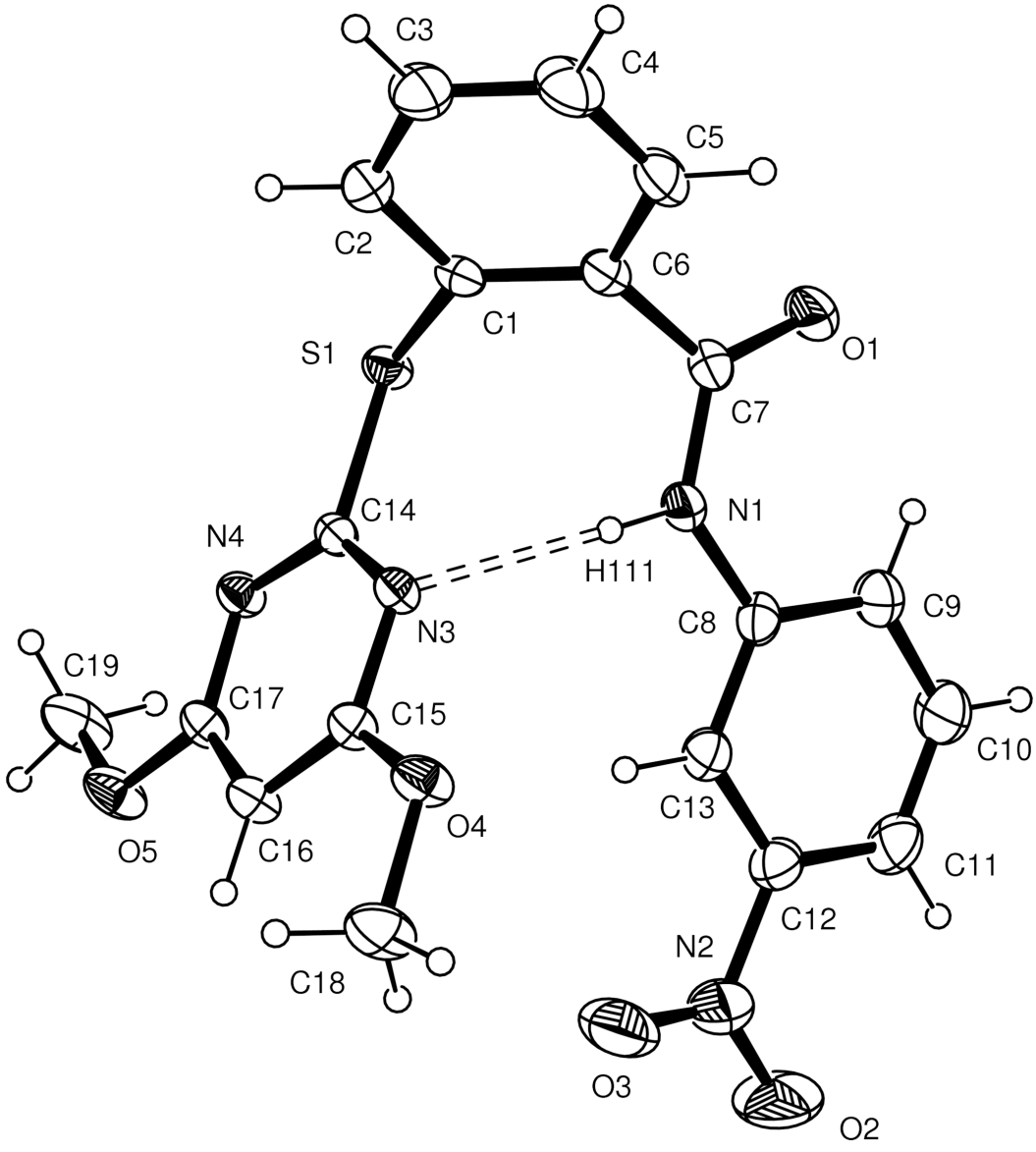
O3—N2	1.216 (3)	C12—C13	1.385 (2)
O4—C15	1.322 (2)	C15—C16	1.364 (2)
O4—C18	1.466 (2)	C16—C17	1.384 (2)
O5—C17	1.329 (2)	N1—H111	0.860
O5—C19	1.431 (2)	C2—H2	0.930
N1—C7	1.374 (2)	C3—H3	0.930
N1—C8	1.414 (2)	C4—H4	0.930
N2—C12	1.488 (3)	C5—H5	0.930
N3—C14	1.308 (2)	C9—H9	0.930
N3—C15	1.373 (2)	C10—H10	0.930
N4—C14	1.329 (2)	C11—H11	0.930
N4—C17	1.353 (2)	C13—H13	0.930
C1—C2	1.396 (2)	C16—H16	0.930
C1—C6	1.383 (2)	C18—H181	0.960
C2—C3	1.373 (3)	C18—H182	0.960
C3—C4	1.350 (3)	C18—H183	0.960
C4—C5	1.379 (3)	C19—H191	0.960
C5—C6	1.379 (2)	C19—H192	0.960
C6—C7	1.515 (2)	C19—H193	0.960
C8—C9	1.409 (2)		
C1—S1—C14	104.39 (8)	N3—C15—C16	123.14 (15)
C15—O4—C18	118.05 (14)	C15—C16—C17	113.49 (16)
C17—O5—C19	115.06 (15)	O5—C17—N4	120.25 (16)
C7—N1—C8	129.00 (15)	O5—C17—C16	114.34 (16)
O2—N2—O3	122.0 (2)	N4—C17—C16	125.41 (16)
O2—N2—C12	118.6 (2)	C7—N1—H111	115.5
O3—N2—C12	119.4 (2)	C8—N1—H111	115.5
C14—N3—C15	117.24 (14)	C1—C2—H2	119.9
C14—N4—C17	114.99 (15)	C3—C2—H2	119.9
S1—C1—C2	116.94 (14)	C2—C3—H3	120.1
S1—C1—C6	122.61 (14)	C4—C3—H3	120.1
C2—C1—C6	119.94 (16)	C3—C4—H4	119.6
C1—C2—C3	120.26 (18)	C5—C4—H4	119.6
C2—C3—C4	119.7 (2)	C4—C5—H5	119.5
C3—C4—C5	120.8 (2)	C6—C5—H5	119.5
C4—C5—C6	120.9 (2)	C8—C9—H9	120.9
C1—C6—C5	118.40 (17)	C10—C9—H9	120.9
C1—C6—C7	124.81 (16)	C9—C10—H10	118.8
C5—C6—C7	116.78 (16)	C11—C10—H10	118.8
O1—C7—N1	125.63 (17)	C10—C11—H11	120.9
O1—C7—C6	121.04 (16)	C12—C11—H11	120.9
N1—C7—C6	113.08 (15)	C8—C13—H13	120.3
N1—C8—C9	122.62 (17)	C12—C13—H13	120.3
N1—C8—C13	117.14 (15)	C15—C16—H16	123.3
C9—C8—C13	120.22 (17)	C17—C16—H16	123.3
C8—C9—C10	118.1 (2)	O4—C18—H181	109.5
C9—C10—C11	122.4 (2)	O4—C18—H182	109.5
C10—C11—C12	118.1 (2)	O4—C18—H183	109.5
N2—C12—C11	119.84 (19)	H181—C18—H182	109.5

N2—C12—C13	118.36 (18)	H181—C18—H183	109.5
C11—C12—C13	121.8 (2)	H182—C18—H183	109.5
C8—C13—C12	119.32 (18)	O5—C19—H191	109.5
S1—C14—N3	120.91 (12)	O5—C19—H192	109.5
S1—C14—N4	113.35 (12)	O5—C19—H193	109.5
N3—C14—N4	125.68 (15)	H191—C19—H192	109.5
O4—C15—N3	113.12 (15)	H191—C19—H193	109.5
O4—C15—C16	123.71 (16)	H192—C19—H193	109.5
C1—S1—C14—N3	−24.72 (16)	C2—C1—C6—C5	−0.5 (2)
C1—S1—C14—N4	157.85 (12)	C2—C1—C6—C7	178.00 (17)
C14—S1—C1—C2	−92.52 (15)	C6—C1—C2—C3	−1.1 (3)
C14—S1—C1—C6	95.79 (16)	C1—C2—C3—C4	1.4 (3)
C18—O4—C15—N3	178.38 (17)	C2—C3—C4—C5	−0.2 (3)
C18—O4—C15—C16	−3.9 (2)	C3—C4—C5—C6	−1.4 (3)
C19—O5—C17—N4	5.0 (2)	C4—C5—C6—C1	1.7 (3)
C19—O5—C17—C16	−175.2 (2)	C4—C5—C6—C7	−176.9 (2)
C7—N1—C8—C9	2.2 (3)	C1—C6—C7—O1	128.8 (2)
C7—N1—C8—C13	−179.17 (18)	C1—C6—C7—N1	−56.6 (2)
C8—N1—C7—O1	−3.7 (3)	C5—C6—C7—O1	−52.7 (2)
C8—N1—C7—C6	−177.95 (16)	C5—C6—C7—N1	121.85 (19)
O2—N2—C12—C11	−4.4 (3)	N1—C8—C9—C10	178.3 (2)
O2—N2—C12—C13	176.9 (2)	N1—C8—C13—C12	−179.31 (18)
O3—N2—C12—C11	174.3 (2)	C9—C8—C13—C12	−0.6 (3)
O3—N2—C12—C13	−4.4 (3)	C13—C8—C9—C10	−0.3 (3)
C14—N3—C15—O4	179.89 (15)	C8—C9—C10—C11	0.9 (3)
C14—N3—C15—C16	2.1 (2)	C9—C10—C11—C12	−0.4 (4)
C15—N3—C14—S1	−178.51 (12)	C10—C11—C12—N2	−179.2 (2)
C15—N3—C14—N4	−1.4 (2)	C10—C11—C12—C13	−0.5 (3)
C14—N4—C17—O5	−178.28 (16)	N2—C12—C13—C8	179.73 (19)
C14—N4—C17—C16	2.0 (2)	C11—C12—C13—C8	1.1 (3)
C17—N4—C14—S1	176.74 (12)	O4—C15—C16—C17	−178.33 (16)
C17—N4—C14—N3	−0.5 (2)	N3—C15—C16—C17	−0.8 (2)
S1—C1—C2—C3	−172.99 (18)	C15—C16—C17—O5	178.93 (16)
S1—C1—C6—C5	170.98 (16)	C15—C16—C17—N4	−1.4 (2)
S1—C1—C6—C7	−10.6 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N(1)—H(111)···N(3)	0.860	2.098	2.914 (2)	158.2

Fig. 1


C3
C4
C5
C2
C6
C1
S1
O1
C7
C14
N1
N4
H111
C8
C9
N3
C19
C17
C15
C10
C13
O5
C16
O4
C11
C12
N2
C18
O3
O2