Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Amino-*N*-(6-chloro-5-methoxypyrimidin-4-yl)benzenesulfonamide

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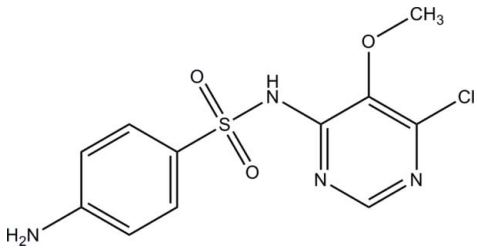
Received 5 January 2010; accepted 9 January 2010

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.030; wR factor = 0.089; data-to-parameter ratio = 21.6.

In the title compound, $C_{11}H_{11}ClN_4O_3S$, the S atom is bonded in a distorted tetrahedral geometry, by two O atoms, a C atom of the benzene ring and an amino N atom. The essentially planar pyrimidine ring [maximum deviation = 0.020 (1) Å] forms a dihedral angle of 87.57 (5)° with the benzene ring. In the crystal structure, pairs of molecules are linked by intermolecular N—H···O hydrogen bonds to generate centrosymmetric $R_2^2(8)$ ring motifs. In addition, molecules are linked into a three-dimensional extended network by intermolecular N—H···N, N—H···O and C—H···O hydrogen bonds.

Related literature

For general background to and applications of the title compound, see: Amir *et al.* (2007); Calabresi *et al.* (1975); El-Hashash *et al.* (1993); Nagaraja *et al.* (2003); Townsend & Drach (2002). For a related structure, see: Chohan *et al.* (2008). For details of hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).



‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: C-7576-2009.

Experimental

Crystal data

$C_{11}H_{11}ClN_4O_3S$
M_r = 314.75
Monoclinic, $P2_1/c$
a = 12.8792 (6) Å
b = 13.3557 (6) Å
c = 8.0867 (4) Å
β = 102.396 (1)°
V = 1358.57 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 100 K
0.44 × 0.33 × 0.12 mm

Data collection

Bruker SMART APEX DUO area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.829, T_{max} = 0.950
20122 measured reflections
4863 independent reflections
4292 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.089
S = 1.04
4863 reflections
225 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*1···N4^{i}	0.875 (19)	2.616 (18)	3.4230 (14)	153.8 (15)
N1—H2*N*1···O1^{ii}	0.882 (18)	2.533 (19)	3.3274 (13)	150.2 (15)
N2—H1*N*2···O2^{iii}	0.880 (18)	2.031 (18)	2.8866 (12)	163.7 (16)
C4—H4*A*···O1^{ii}	0.944 (16)	2.460 (16)	3.2603 (13)	142.5 (13)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $x, y, z+1$; (iii) $-x, -y+1, -z+2$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HKF and JHG thank Universiti Sains Malaysia (USM) for the Research University Golden Goose grant (No. 1001/PFIZIK/811012). JHG also thanks USM for the award of a USM fellowship. CSC thanks the University of Mysore for research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2975).

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supporting information

Acta Cryst. (2010). E**66**, o372–o373 [https://doi.org/10.1107/S1600536810001121]

4-Amino-*N*-(6-chloro-5-methoxypyrimidin-4-yl)benzenesulfonamide

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S1. Comment

The importance of pyrimidines and analogous compounds in pharmaceutical and biological fields is well known (Townsend *et al.*, 2002). Some substituted pyrimidines and their derivaties have been reported to possess anti-microbial and anti-fungal activities (El-Hashash *et al.*, 1993). Pyrimidines have incidental anti-viral activity against herpes and vaccinia infections (Calabresi *et al.*, 1975). A review on pyrimidines as anti-inflammatory agent is described by Amir *et al.* (2007). Sulfonamides are an important class of anti-bacterial drugs used in medicine and veterinary practice. Sulfa drugs are widely used in the treatment of infections, especially for patients intolerant to antibiotics. The vast commercial success of these medicinal agents has made the chemistry of sulfonamides to become a major area of research and an important branch of commercial importance in pharmaceutical sciences (Nagaraja *et al.*, 2003). In view of the importance of the title compound possessing potential anti-bacterial properties, its crystal structure is reported herein.

In the title sulfonamide compound (Fig. 1), the geometry around the S1 atom is a distorted tetrahedron, comprising of atoms O1 and O2 of the sulfonyl group, C6 atom of benzene ring and the amino atom N2. The O1–S1–O2 and O2–S1–N2 angles are 119.20 (5) and 102.20 (4)°, respectively, and the C6–S1–N2–C7 torsion angle is -68.95 (9)°. The pyrimidine ring is essentially planar, with r.m.s. deviation of -0.020 (1) Å, and is almost perpendicular to the benzene ring (C1-C6), as indicated by the dihedral angle of 87.57 (5)°. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to a related structure (Chohan *et al.*, 2008). In the crystal structure, pairs of intermolecular N2—H1N2···O2^{iii} hydrogen bonds (see Table 1 for symmetry code) generate $R^2_2(8)$ ring motifs (Bernstein *et al.*, 1995). Neighbouring molecules are linked into a three-dimensional extended network by intermolecular N1—H1N1···N4, N1—H2N1···O1 and C4—H4A···O1 hydrogen bonds (Fig. 2).

S2. Experimental

The title compound was obtained as a gift sample from R. L. Fine Chem, Bangalore, India. The compound was used without further purification. Single crystals of good quality were obtained from slow evaporation of an acetonitrile solution. *M.p.* 447–450 K.

S3. Refinement

All the H atoms were located in a difference Fourier map and allowed to refine freely [range of C—H = 0.90 (2) - 0.991 (19) Å].

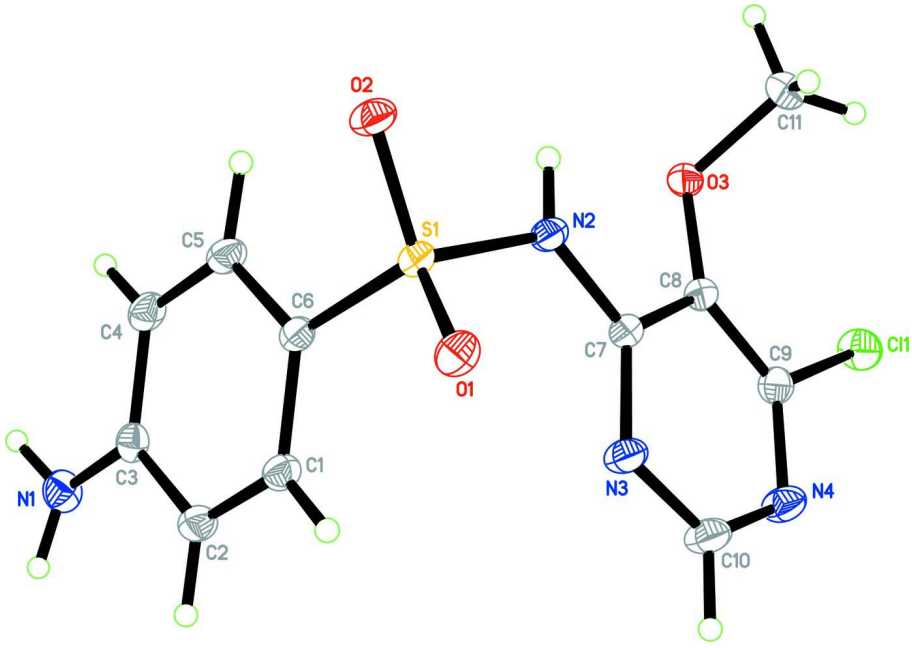

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids for non-H atoms and the atom-numbering scheme.

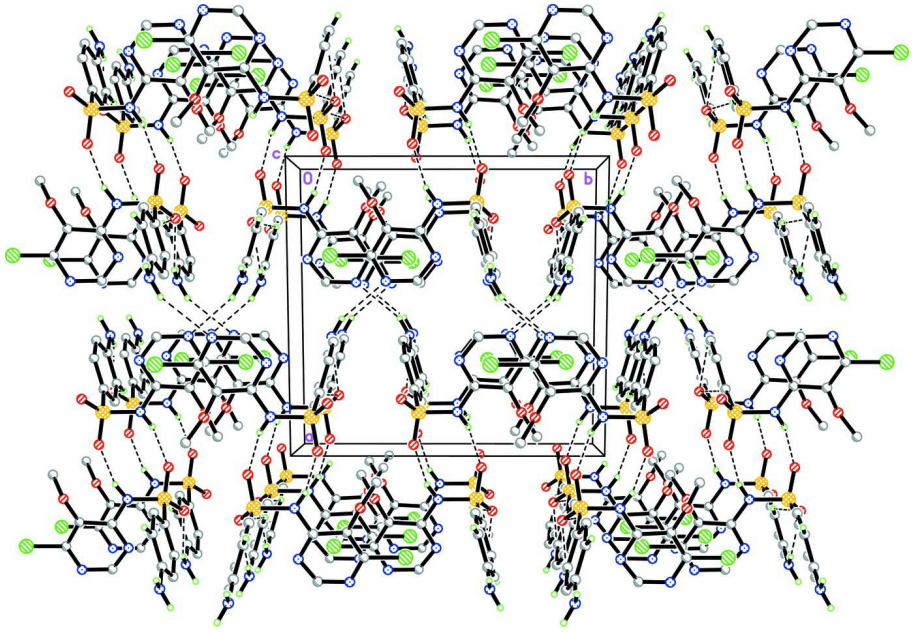

Figure 2

Part of the crystal structure of the title compound, viewed along the *c* axis, showing a three-dimensional extended network. H atoms not involved in intermolecular hydrogen bonds (dashed lines) have been omitted for clarity.

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Crystal data

$C_{11}H_{11}ClN_4O_3S$
$M_r = 314.75$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.8792$ (6) Å
$b = 13.3557$ (6) Å
$c = 8.0867$ (4) Å
$\beta = 102.396$ (1)°
$V = 1358.57$ (11) Å^3
$Z = 4$
$F(000) = 648$
$D_x = 1.539$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9451 reflections
$\theta = 3.1$–$35.0°$
$\mu = 0.45$ mm^{-1}
$T = 100$ K
Plate, colourless
0.44 × 0.33 × 0.12 mm

Data collection

Bruker SMART APEX DUO area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.829$, $T_{max} = 0.950$
20122 measured reflections
4863 independent reflections
4292 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 32.5°$, $\theta_{min} = 1.6°$
$h = -19 \rightarrow 18$
$k = -20 \rightarrow 20$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.089$
$S = 1.04$
4863 reflections
225 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.4528P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.32221 (2)	0.130087 (19)	0.89383 (4)	0.02300 (7)
S1	0.150384 (18)	0.591224 (17)	0.98106 (3)	0.01312 (6)

O1	0.19845 (6)	0.64388 (6)	0.86316 (9)	0.01714 (14)
O2	0.03978 (6)	0.60773 (6)	0.97922 (10)	0.01793 (14)
O3	0.15020 (6)	0.26617 (6)	0.97198 (9)	0.01711 (14)
N1	0.40417 (8)	0.62924 (7)	1.67597 (11)	0.02030 (18)
N2	0.15327 (7)	0.46898 (6)	0.94120 (11)	0.01577 (15)
N3	0.32756 (7)	0.46232 (7)	0.89578 (12)	0.01792 (16)
N4	0.40819 (7)	0.30443 (7)	0.86117 (13)	0.01997 (17)
C1	0.32974 (8)	0.63720 (7)	1.21150 (12)	0.01551 (17)
C2	0.38928 (8)	0.64543 (8)	1.37493 (13)	0.01691 (17)
C3	0.34401 (8)	0.62413 (7)	1.51452 (12)	0.01546 (17)
C4	0.23638 (8)	0.59518 (8)	1.48550 (13)	0.01756 (18)
C5	0.17708 (8)	0.58676 (8)	1.32262 (13)	0.01685 (18)
C6	0.22376 (7)	0.60750 (7)	1.18497 (12)	0.01355 (16)
C7	0.24116 (7)	0.41496 (7)	0.92115 (12)	0.01407 (16)
C8	0.23504 (7)	0.30973 (7)	0.92579 (12)	0.01413 (16)
C9	0.32214 (8)	0.25928 (7)	0.89322 (12)	0.01631 (17)
C10	0.40614 (8)	0.40413 (8)	0.86664 (15)	0.0207 (2)
C11	0.07329 (9)	0.21978 (10)	0.83669 (16)	0.0253 (2)
H1A	0.3591 (13)	0.6546 (12)	1.120 (2)	0.025 (4)*
H2A	0.4615 (13)	0.6672 (13)	1.393 (2)	0.027 (4)*
H4A	0.2078 (13)	0.5806 (12)	1.581 (2)	0.027 (4)*
H5A	0.1038 (13)	0.5624 (12)	1.303 (2)	0.026 (4)*
H10A	0.4693 (14)	0.4379 (13)	0.847 (2)	0.030 (4)*
H11A	0.0146 (14)	0.2042 (14)	0.883 (2)	0.035 (4)*
H11B	0.0532 (14)	0.2688 (14)	0.743 (2)	0.038 (5)*
H11C	0.0991 (15)	0.1654 (16)	0.795 (2)	0.043 (5)*
H1N1	0.4646 (14)	0.6617 (14)	1.695 (2)	0.033 (4)*
H2N1	0.3696 (15)	0.6271 (14)	1.759 (2)	0.034 (5)*
H1N2	0.1012 (14)	0.4342 (13)	0.968 (2)	0.030 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.02251 (13)	0.01320 (11)	0.03324 (15)	0.00115 (8)	0.00591 (10)	−0.00126 (9)
S1	0.01184 (10)	0.01368 (11)	0.01457 (11)	0.00149 (7)	0.00442 (8)	0.00027 (7)
O1	0.0191 (3)	0.0179 (3)	0.0156 (3)	0.0009 (3)	0.0064 (3)	0.0026 (2)
O2	0.0121 (3)	0.0195 (3)	0.0228 (3)	0.0032 (2)	0.0050 (3)	0.0005 (3)
O3	0.0161 (3)	0.0188 (3)	0.0177 (3)	−0.0056 (3)	0.0064 (3)	−0.0027 (3)
N1	0.0241 (4)	0.0228 (4)	0.0140 (4)	−0.0020 (3)	0.0041 (3)	−0.0002 (3)
N2	0.0129 (3)	0.0139 (3)	0.0220 (4)	−0.0005 (3)	0.0071 (3)	−0.0028 (3)
N3	0.0143 (4)	0.0154 (4)	0.0260 (4)	0.0000 (3)	0.0085 (3)	−0.0005 (3)
N4	0.0161 (4)	0.0172 (4)	0.0285 (4)	0.0019 (3)	0.0091 (3)	0.0003 (3)
C1	0.0155 (4)	0.0164 (4)	0.0160 (4)	−0.0008 (3)	0.0063 (3)	0.0003 (3)
C2	0.0159 (4)	0.0189 (4)	0.0167 (4)	−0.0015 (3)	0.0053 (3)	0.0000 (3)
C3	0.0191 (4)	0.0130 (4)	0.0148 (4)	0.0011 (3)	0.0049 (3)	−0.0002 (3)
C4	0.0202 (4)	0.0185 (4)	0.0161 (4)	−0.0004 (3)	0.0087 (3)	0.0009 (3)
C5	0.0157 (4)	0.0188 (4)	0.0178 (4)	−0.0007 (3)	0.0076 (3)	0.0008 (3)
C6	0.0135 (4)	0.0136 (4)	0.0145 (4)	0.0006 (3)	0.0049 (3)	0.0000 (3)

C7	0.0123 (4)	0.0149 (4)	0.0154 (4)	0.0003 (3)	0.0041 (3)	−0.0017 (3)
C8	0.0137 (4)	0.0148 (4)	0.0144 (4)	−0.0013 (3)	0.0041 (3)	−0.0010 (3)
C9	0.0167 (4)	0.0135 (4)	0.0189 (4)	0.0011 (3)	0.0042 (3)	−0.0011 (3)
C10	0.0153 (4)	0.0180 (4)	0.0313 (5)	0.0004 (3)	0.0103 (4)	−0.0002 (4)
C11	0.0196 (5)	0.0299 (6)	0.0268 (5)	−0.0086 (4)	0.0058 (4)	−0.0109 (4)

Geometric parameters (Å, º)

Cl1—C9	1.7255 (10)	C1—C2	1.3826 (14)
S1—O1	1.4283 (7)	C1—C6	1.3932 (13)
S1—O2	1.4383 (7)	C1—H1A	0.931 (16)
S1—N2	1.6662 (9)	C2—C3	1.4063 (13)
S1—C6	1.7292 (10)	C2—H2A	0.955 (17)
O3—C8	1.3590 (11)	C3—C4	1.4094 (14)
O3—C11	1.4480 (13)	C4—C5	1.3781 (15)
N1—C3	1.3694 (13)	C4—H4A	0.941 (17)
N1—H1N1	0.875 (18)	C5—C6	1.4016 (13)
N1—H2N1	0.879 (19)	C5—H5A	0.979 (16)
N2—C7	1.3809 (12)	C7—C8	1.4085 (14)
N2—H1N2	0.880 (18)	C8—C9	1.3816 (13)
N3—C7	1.3336 (12)	C10—H10A	0.973 (17)
N3—C10	1.3364 (13)	C11—H11A	0.938 (18)
N4—C10	1.3328 (14)	C11—H11B	0.991 (19)
N4—C9	1.3351 (13)	C11—H11C	0.90 (2)
O1—S1—O2	119.20 (5)	C3—C4—H4A	117.7 (10)
O1—S1—N2	108.81 (4)	C4—C5—C6	119.92 (9)
O2—S1—N2	102.20 (4)	C4—C5—H5A	119.9 (10)
O1—S1—C6	110.38 (5)	C6—C5—H5A	120.1 (10)
O2—S1—C6	109.14 (5)	C1—C6—C5	120.47 (9)
N2—S1—C6	106.10 (5)	C1—C6—S1	119.96 (7)
C8—O3—C11	115.81 (8)	C5—C6—S1	119.52 (8)
C3—N1—H1N1	119.3 (12)	N3—C7—N2	120.16 (9)
C3—N1—H2N1	116.6 (12)	N3—C7—C8	122.05 (9)
H1N1—N1—H2N1	117.5 (17)	N2—C7—C8	117.78 (8)
C7—N2—S1	125.98 (7)	O3—C8—C9	125.25 (9)
C7—N2—H1N2	116.1 (11)	O3—C8—C7	119.17 (8)
S1—N2—H1N2	114.8 (11)	C9—C8—C7	115.41 (9)
C7—N3—C10	116.09 (9)	N4—C9—C8	123.96 (9)
C10—N4—C9	114.94 (9)	N4—C9—Cl1	116.89 (7)
C2—C1—C6	119.60 (9)	C8—C9—Cl1	119.15 (8)
C2—C1—H1A	120.2 (10)	N4—C10—N3	127.44 (10)
C6—C1—H1A	120.1 (10)	N4—C10—H10A	115.8 (10)
C1—C2—C3	120.71 (9)	N3—C10—H10A	116.8 (10)
C1—C2—H2A	119.7 (10)	O3—C11—H11A	105.7 (11)
C3—C2—H2A	119.6 (10)	O3—C11—H11B	108.5 (11)
N1—C3—C2	120.53 (9)	H11A—C11—H11B	110.6 (15)
N1—C3—C4	120.49 (9)	O3—C11—H11C	112.6 (12)

C2—C3—C4	118.96 (9)	H11A—C11—H11C	111.6 (17)
C5—C4—C3	120.34 (9)	H11B—C11—H11C	107.8 (16)
C5—C4—H4A	122.0 (10)		
O1—S1—N2—C7	49.81 (10)	C10—N3—C7—N2	−175.76 (10)
O2—S1—N2—C7	176.75 (8)	C10—N3—C7—C8	3.19 (15)
C6—S1—N2—C7	−68.95 (9)	S1—N2—C7—N3	−14.89 (14)
C6—C1—C2—C3	0.01 (15)	S1—N2—C7—C8	166.11 (7)
C1—C2—C3—N1	177.89 (10)	C11—O3—C8—C9	−78.05 (13)
C1—C2—C3—C4	−0.66 (15)	C11—O3—C8—C7	106.84 (11)
N1—C3—C4—C5	−177.74 (10)	N3—C7—C8—O3	172.23 (9)
C2—C3—C4—C5	0.80 (15)	N2—C7—C8—O3	−8.80 (13)
C3—C4—C5—C6	−0.30 (15)	N3—C7—C8—C9	−3.36 (14)
C2—C1—C6—C5	0.51 (15)	N2—C7—C8—C9	175.62 (9)
C2—C1—C6—S1	−176.93 (8)	C10—N4—C9—C8	1.60 (15)
C4—C5—C6—C1	−0.37 (15)	C10—N4—C9—Cl1	−178.19 (8)
C4—C5—C6—S1	177.08 (8)	O3—C8—C9—N4	−174.46 (10)
O1—S1—C6—C1	−20.24 (9)	C7—C8—C9—N4	0.82 (14)
O2—S1—C6—C1	−153.06 (8)	O3—C8—C9—Cl1	5.32 (14)
N2—S1—C6—C1	97.49 (8)	C7—C8—C9—Cl1	−179.40 (7)
O1—S1—C6—C5	162.29 (8)	C9—N4—C10—N3	−1.89 (18)
O2—S1—C6—C5	29.47 (9)	C7—N3—C10—N4	−0.47 (18)
N2—S1—C6—C5	−79.98 (9)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···N4^{i}	0.875 (19)	2.616 (18)	3.4230 (14)	153.8 (15)
N1—H2*N*1···O1^{ii}	0.882 (18)	2.533 (19)	3.3274 (13)	150.2 (15)
N2—H1*N*2···O2^{iii}	0.880 (18)	2.031 (18)	2.8866 (12)	163.7 (16)
C4—H4*A*···O1^{ii}	0.944 (16)	2.460 (16)	3.2603 (13)	142.5 (13)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+5/2; (ii) *x*, *y*, *z*+1; (iii) −*x*, −*y*+1, −*z*+2.