Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chloro-1,3-benzothiazol-2-yl)-2-(3-methylphenyl)acetamide monohydrate

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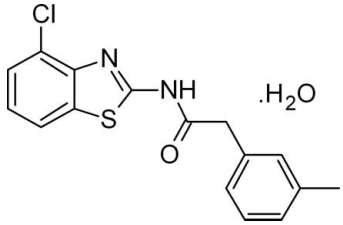
Received 30 August 2011; accepted 2 September 2011

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.089; data-to-parameter ratio = 20.6.

In the title compound, $C_{16}H_{13}ClN_2OS\cdot H_2O$, the dihedral angle between the mean planes of the benzothiazole ring system and the methylphenyl ring is 79.3 (6)°. The crystal packing features intermolecular O—H···N, O—H···O and N—H···O hydrogen bonds involving the water molecule and weak C—H···O, C—H···*Cg* and π–π stacking interactions [centroid–centroid distances = 3.8743 (7), 3.7229 (7) and 3.7076 (8) Å].

Related literature

For the biological activity of compounds with benzothiazole skeletons, see: Aiello *et al.* (2008); Cho *et al.* (2008). For their structural similarity to the lateral chain of natural benzylpenicillin, see: Mijin & Marinkovic (2006); Mijin *et al.* (2006, 2008) and for their coordination abilities, see: Wu *et al.* (2008, 2010). For related structures, see: Davis & Healy (2010); John *et al.* (2010); Nogueira *et al.* (2010); Praveen *et al.* (2011); Selig *et al.* (2010); Wen *et al.* (2010); Xiao *et al.* (2010). For standard bond lengths, see Allen *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{13}ClN_2OS\cdot H_2O$
M_r = 334.81
Triclinic, $P\overline{1}$
a = 7.2771 (3) Å
b = 9.2568 (5) Å
c = 12.0851 (5) Å
α = 83.948 (4)°
β = 84.306 (3)°
γ = 72.133 (4)°
V = 768.58 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 173 K
0.25 × 0.21 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.908, T_{max} = 0.926
10307 measured reflections
4303 independent reflections
3834 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.089
S = 1.01
4303 reflections
209 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*OB*···N1^{i}	0.88 (1)	2.10 (2)	2.924 (1)	158 (2)
O2—H2*OA*···O1^{ii}	0.88 (1)	2.05 (1)	2.904 (1)	164 (2)
N2—H2*N*···O2	0.87 (1)	1.92 (1)	2.785 (1)	177 (2)
C5—H5*A*···O1^{iii}	0.95	2.56	3.351 (2)	141
C3—H3*A*···*Cg*3^{iv}	0.95	2.66	3.502 (1)	148

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); 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*.

ASP and HSY thank the UoM for research facilities. JPJ acknowledges the NSF–MRI program (grant No. CHE1039027) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2316).

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supporting information

Acta Cryst. (2011). E**67**, o2602–o2603 [https://doi.org/10.1107/S1600536811035872]

N-(4-Chloro-1,3-benzothiazol-2-yl)-2-(3-methylphenyl)acetamide monohydrate

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S1. Comment

The biological activity of compounds with benzothiazole skeletons includes anticancer, antibacterial, antifungal and anthelmintic properties (Aiello *et al.*, 2008; Cho *et al.*, 2008) N-Substituted 2-arylacetamides are very interesting compounds because of their structural similarity to the lateral chain of natural benzylpenicillin (Mijin *et al.*, 2008; Mijin *et al.*, 2006). Amides are also used as ligands due to their excellent coordination abilities (Wu *et al.*, 2008; 2010). Crystal structures of some acetamidederivatives, viz., 2-(4-bromophenyl)-N-(2-methoxyphenyl)acetamide (Xiao *et al.*, 2010), N-benzyl-2-(3-chloro-4-hydroxyphenyl)acetamide (Davis *et al.*, 2010), 2-[(5,7-dibromoquinolin-8-yl)oxy]-N-(2-methoxyphenyl)acetamide (Wen *et al.*, 2010), N-(4-bromophenyl)-2-(2-thienyl)acetamide (Nogueira *et al.*, 2010), N-[4-(benzylsulfamoyl)phenyl]acetamide (John *et al.*, 2010), 2-(4-fluorophenyl)-N-{4-[6-(4-fluorophenyl)-2,3-dihydroimidazo[2,1-b][1,3] thiazol-5-yl]pyridin-2-yl}acetamide (Selig *et al.*, 2010) and N-(3-chloro-4-fluorophenyl)-2-(naphthalen-1-yl)acetamide (Praveen *et al.*, 2011) have been reported. As part of our ongoing studies of amides, the title compound is synthesized and its crystal structure is reported.

In the title hydrated compound, $C_{16}H_{13}ClN_2OS \times H_2O$, the dihedral angle between the mean planes of the benzothiazole and benzenes is 79.3 (6)° (Fig. 1). Crystal packing is realized by O–H···N, O—H···O and N—H···O hydrogen bonds involving the water molecule and weak O—H···O, C—H···O, C—H···Cg (Table 1) and π–π stacking (Table 2) intermolecular interactions (Fig. 2).

S2. Experimental

To a stirred solution of (3-methylphenyl)acetic acid (1 g, 6.65 mmol), triethylamine (1.34 g, 13.31 mmol) and 4-chloro-1,3-benzothiazol-2-amine (1.27 g, 6.65 mmol) in dichloromethane (10 ml), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide HCl (1.52 g, 7.93 mmol) was added at 273 K. The reaction mixture was stirred at room temperature for 3 h. After the completion of the reaction, the reaction mixture was poured into ice cold water and the layers were separated. The organic layer was washed with 10% aq. $NaHCO_3$ solution (10 ml), brine (10 ml), dried over anhydrous Na_2SO_4, filtered and concentrated under vacuum to obtain the crude product which was triturated with ethanol and filtered to afford 1.92 g of the title compound (I) as a white solid in 91 % yield. Single crystals were grown from ethanol by slow evaporation method (m.p.: 397-398 K).

S3. Refinement

H20A, H20B and H2N were located by a Fourier map and refined isotropically. All other H atoms were placed in their calculated positions and then refined using the riding model with atom—H lengths of 0.95Å (CH), 0.99Å (CH_2) or 0.98Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.18-1.21 (CH) 1.20 CH_2) or 1.51 (CH_3) times U_{eq} of the parent atom.

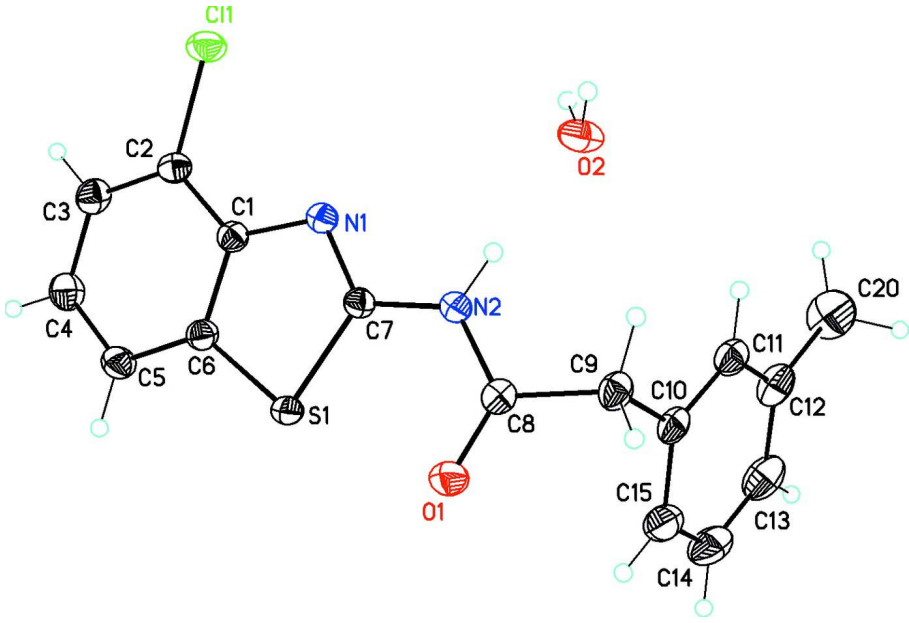

Figure 1

Molecular structure of the title compound showing the atom labeling scheme and 30% probability displacement ellipsoids.

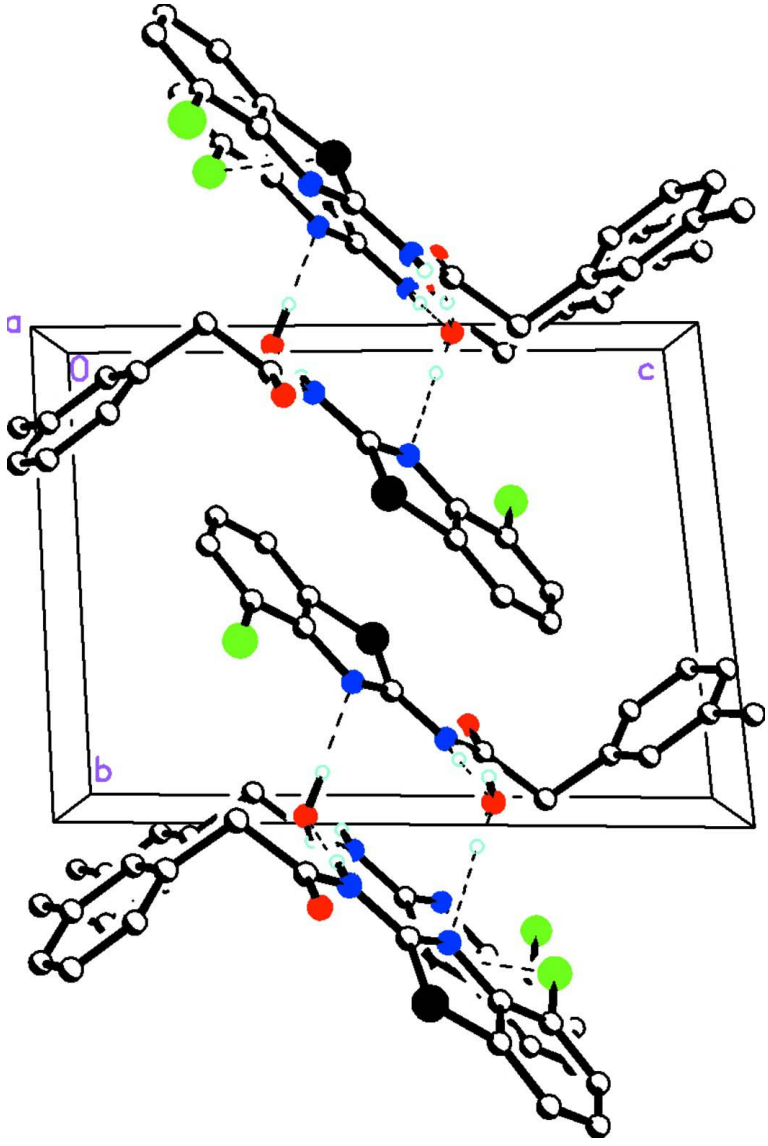

Figure 2

Packing diagram of the title compound viewed down the *a* axis. Dashed lines indicate O—H···N hydrogen bonds.

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Crystal data

$C_{16}H_{13}ClN_2OS·H_2O$
$M_r = 334.81$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2771\ (3)$ Å
$b = 9.2568\ (5)$ Å
$c = 12.0851\ (5)$ Å
$\alpha = 83.948\ (4)°$
$\beta = 84.306\ (3)°$
$\gamma = 72.133\ (4)°$
$V = 768.58\ (6)$ Å^3

$Z = 2$
$F(000) = 348$
$D_x = 1.447$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5935 reflections
$\theta = 3.2–32.2°$
$\mu = 0.39$ mm^{-1}
$T = 173$ K
Block, colorless
0.25 × 0.21 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 16.1500 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.908, T_{max} = 0.926
10307 measured reflections
4303 independent reflections
3834 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 29.6°, θ_{min} = 3.2°
h = −6→10
k = −12→12
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.089
S = 1.01
4303 reflections
209 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.2662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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. 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
S1	0.10411 (4)	0.65402 (3)	0.47845 (2)	0.02017 (8)
Cl1	0.78434 (4)	0.64763 (4)	0.28146 (3)	0.02807 (9)
O1	−0.10370 (13)	0.84965 (11)	0.62242 (8)	0.02685 (19)
O2	0.47923 (14)	0.98584 (11)	0.64369 (9)	0.0289 (2)
H2OB	0.477 (2)	1.0762 (16)	0.6127 (14)	0.035*
H2OA	0.600 (2)	0.9272 (17)	0.6380 (15)	0.035*
N1	0.41640 (14)	0.74054 (11)	0.44287 (8)	0.01894 (19)
N2	0.19872 (14)	0.86818 (11)	0.58166 (8)	0.01959 (19)
H2N	0.285 (2)	0.9074 (18)	0.5985 (13)	0.024*
C1	0.43805 (16)	0.62472 (13)	0.37390 (9)	0.0181 (2)
C2	0.59653 (16)	0.56742 (13)	0.29843 (10)	0.0202 (2)
C3	0.60131 (18)	0.44952 (14)	0.23612 (11)	0.0242 (2)
H3A	0.7097	0.4102	0.1856	0.029*
C4	0.44702 (19)	0.38796 (14)	0.24728 (11)	0.0263 (3)
H4A	0.4525	0.3063	0.2043	0.032*

C5	0.28611 (18)	0.44326 (14)	0.31952 (11)	0.0237 (2)
H5A	0.1808	0.4018	0.3261	0.028*
C6	0.28419 (17)	0.56185 (13)	0.38211 (9)	0.0195 (2)
C7	0.25131 (16)	0.76327 (13)	0.50223 (9)	0.0179 (2)
C8	0.02371 (17)	0.90296 (13)	0.64119 (10)	0.0200 (2)
C9	0.00054 (18)	1.00506 (14)	0.73487 (10)	0.0224 (2)
H9A	−0.1334	1.0745	0.7408	0.027*
H9B	0.0903	1.0675	0.7194	0.027*
C10	0.04473 (18)	0.90619 (14)	0.84323 (10)	0.0219 (2)
C11	0.20475 (18)	0.90263 (15)	0.89814 (10)	0.0246 (2)
H11A	0.2826	0.9654	0.8689	0.030*
C12	0.2537 (2)	0.80858 (16)	0.99563 (11)	0.0303 (3)
C13	0.1374 (2)	0.71844 (17)	1.03722 (12)	0.0348 (3)
H13A	0.1688	0.6535	1.1033	0.042*
C14	−0.0235 (2)	0.72173 (17)	0.98378 (12)	0.0347 (3)
H14A	−0.1020	0.6597	1.0137	0.042*
C15	−0.0708 (2)	0.81538 (16)	0.88651 (11)	0.0287 (3)
H15A	−0.1813	0.8174	0.8498	0.034*
C20	0.4298 (2)	0.8049 (2)	1.05269 (14)	0.0455 (4)
H20A	0.5070	0.6990	1.0692	0.068*
H20B	0.3894	0.8551	1.1224	0.068*
H20C	0.5076	0.8584	1.0037	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01938 (14)	0.02259 (14)	0.02136 (14)	−0.01061 (11)	0.00229 (10)	−0.00472 (10)
Cl1	0.02011 (15)	0.03273 (17)	0.03346 (17)	−0.01163 (12)	0.00420 (11)	−0.00644 (12)
O1	0.0204 (4)	0.0311 (5)	0.0311 (5)	−0.0101 (4)	0.0026 (3)	−0.0085 (4)
O2	0.0231 (4)	0.0243 (4)	0.0412 (5)	−0.0111 (4)	0.0024 (4)	−0.0034 (4)
N1	0.0190 (4)	0.0195 (4)	0.0197 (4)	−0.0079 (4)	0.0003 (3)	−0.0030 (4)
N2	0.0192 (5)	0.0215 (5)	0.0203 (4)	−0.0089 (4)	0.0008 (4)	−0.0049 (4)
C1	0.0190 (5)	0.0172 (5)	0.0181 (5)	−0.0056 (4)	−0.0012 (4)	−0.0004 (4)
C2	0.0175 (5)	0.0202 (5)	0.0221 (5)	−0.0054 (4)	−0.0003 (4)	−0.0004 (4)
C3	0.0225 (6)	0.0219 (5)	0.0260 (6)	−0.0035 (4)	0.0021 (4)	−0.0055 (4)
C4	0.0288 (6)	0.0209 (5)	0.0293 (6)	−0.0066 (5)	0.0007 (5)	−0.0081 (5)
C5	0.0247 (6)	0.0220 (5)	0.0269 (6)	−0.0103 (5)	0.0003 (4)	−0.0052 (4)
C6	0.0197 (5)	0.0193 (5)	0.0199 (5)	−0.0069 (4)	0.0005 (4)	−0.0017 (4)
C7	0.0189 (5)	0.0181 (5)	0.0177 (5)	−0.0074 (4)	−0.0013 (4)	−0.0009 (4)
C8	0.0206 (5)	0.0181 (5)	0.0200 (5)	−0.0045 (4)	−0.0007 (4)	−0.0005 (4)
C9	0.0256 (6)	0.0188 (5)	0.0213 (5)	−0.0046 (4)	0.0018 (4)	−0.0039 (4)
C10	0.0235 (5)	0.0200 (5)	0.0197 (5)	−0.0034 (4)	0.0041 (4)	−0.0048 (4)
C11	0.0240 (6)	0.0243 (6)	0.0235 (5)	−0.0047 (5)	0.0032 (4)	−0.0052 (4)
C12	0.0282 (6)	0.0319 (7)	0.0245 (6)	−0.0002 (5)	0.0015 (5)	−0.0032 (5)
C13	0.0387 (8)	0.0317 (7)	0.0259 (6)	−0.0027 (6)	0.0045 (5)	0.0040 (5)
C14	0.0375 (8)	0.0315 (7)	0.0327 (7)	−0.0120 (6)	0.0100 (6)	0.0018 (5)
C15	0.0274 (6)	0.0299 (6)	0.0284 (6)	−0.0096 (5)	0.0044 (5)	−0.0032 (5)
C20	0.0377 (8)	0.0574 (11)	0.0365 (8)	−0.0071 (8)	−0.0108 (6)	0.0042 (7)

Geometric parameters (Å, º)

S1—C6	1.7382 (12)	C5—H5A	0.9500
S1—C7	1.7436 (12)	C8—C9	1.5144 (16)
Cl1—C2	1.7310 (12)	C9—C10	1.5186 (17)
O1—C8	1.2250 (15)	C9—H9A	0.9900
O2—H2OB	0.876 (13)	C9—H9B	0.9900
O2—H2OA	0.883 (13)	C10—C11	1.3866 (18)
N1—C7	1.3068 (15)	C10—C15	1.3934 (18)
N1—C1	1.3884 (14)	C11—C12	1.3963 (18)
N2—C8	1.3633 (15)	C11—H11A	0.9500
N2—C7	1.3809 (14)	C12—C13	1.387 (2)
N2—H2N	0.868 (13)	C12—C20	1.504 (2)
C1—C2	1.4004 (15)	C13—C14	1.383 (2)
C1—C6	1.4028 (16)	C13—H13A	0.9500
C2—C3	1.3799 (17)	C14—C15	1.391 (2)
C3—C4	1.3964 (18)	C14—H14A	0.9500
C3—H3A	0.9500	C15—H15A	0.9500
C4—C5	1.3853 (17)	C20—H20A	0.9800
C4—H4A	0.9500	C20—H20B	0.9800
C5—C6	1.3932 (16)	C20—H20C	0.9800
C6—S1—C7	88.18 (5)	C8—C9—C10	108.76 (10)
H2OB—O2—H2OA	107.2 (14)	C8—C9—H9A	109.9
C7—N1—C1	109.19 (10)	C10—C9—H9A	109.9
C8—N2—C7	123.21 (10)	C8—C9—H9B	109.9
C8—N2—H2N	118.6 (10)	C10—C9—H9B	109.9
C7—N2—H2N	118.0 (11)	H9A—C9—H9B	108.3
N1—C1—C2	126.10 (11)	C11—C10—C15	119.52 (12)
N1—C1—C6	115.52 (10)	C11—C10—C9	119.83 (11)
C2—C1—C6	118.38 (11)	C15—C10—C9	120.63 (12)
C3—C2—C1	120.19 (11)	C10—C11—C12	121.27 (13)
C3—C2—Cl1	120.05 (9)	C10—C11—H11A	119.4
C1—C2—Cl1	119.75 (9)	C12—C11—H11A	119.4
C2—C3—C4	120.06 (11)	C13—C12—C11	118.40 (14)
C2—C3—H3A	120.0	C13—C12—C20	121.33 (14)
C4—C3—H3A	120.0	C11—C12—C20	120.26 (14)
C5—C4—C3	121.51 (11)	C14—C13—C12	120.94 (13)
C5—C4—H4A	119.2	C14—C13—H13A	119.5
C3—C4—H4A	119.2	C12—C13—H13A	119.5
C4—C5—C6	117.62 (11)	C13—C14—C15	120.30 (14)
C4—C5—H5A	121.2	C13—C14—H14A	119.8
C6—C5—H5A	121.2	C15—C14—H14A	119.8
C5—C6—C1	122.21 (11)	C14—C15—C10	119.57 (13)
C5—C6—S1	128.07 (9)	C14—C15—H15A	120.2
C1—C6—S1	109.71 (8)	C10—C15—H15A	120.2
N1—C7—N2	120.77 (10)	C12—C20—H20A	109.5
N1—C7—S1	117.35 (9)	C12—C20—H20B	109.5

N2—C7—S1	121.88 (8)	H20A—C20—H20B	109.5
O1—C8—N2	121.69 (11)	C12—C20—H20C	109.5
O1—C8—C9	122.33 (11)	H20A—C20—H20C	109.5
N2—C8—C9	115.92 (10)	H20B—C20—H20C	109.5
C7—N1—C1—C2	−179.68 (11)	C8—N2—C7—N1	175.97 (11)
C7—N1—C1—C6	0.58 (14)	C8—N2—C7—S1	−5.13 (16)
N1—C1—C2—C3	178.77 (11)	C6—S1—C7—N1	2.23 (10)
C6—C1—C2—C3	−1.50 (17)	C6—S1—C7—N2	−176.71 (10)
N1—C1—C2—Cl1	−2.55 (17)	C7—N2—C8—O1	−4.83 (18)
C6—C1—C2—Cl1	177.18 (9)	C7—N2—C8—C9	172.42 (10)
C1—C2—C3—C4	0.67 (19)	O1—C8—C9—C10	81.73 (14)
Cl1—C2—C3—C4	−178.01 (10)	N2—C8—C9—C10	−95.49 (12)
C2—C3—C4—C5	0.5 (2)	C8—C9—C10—C11	114.28 (12)
C3—C4—C5—C6	−0.8 (2)	C8—C9—C10—C15	−63.84 (14)
C4—C5—C6—C1	−0.11 (19)	C15—C10—C11—C12	0.61 (18)
C4—C5—C6—S1	179.87 (10)	C9—C10—C11—C12	−177.53 (11)
N1—C1—C6—C5	−179.00 (11)	C10—C11—C12—C13	−0.31 (19)
C2—C1—C6—C5	1.24 (18)	C10—C11—C12—C20	179.05 (13)
N1—C1—C6—S1	1.01 (13)	C11—C12—C13—C14	−0.2 (2)
C2—C1—C6—S1	−178.75 (9)	C20—C12—C13—C14	−179.55 (14)
C7—S1—C6—C5	178.34 (12)	C12—C13—C14—C15	0.4 (2)
C7—S1—C6—C1	−1.67 (9)	C13—C14—C15—C10	−0.1 (2)
C1—N1—C7—N2	176.95 (10)	C11—C10—C15—C14	−0.39 (19)
C1—N1—C7—S1	−2.00 (13)	C9—C10—C15—C14	177.73 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*OB*···N1^{i}	0.88 (1)	2.10 (2)	2.924 (1)	158 (2)
O2—H2*OA*···O1^{ii}	0.88 (1)	2.05 (1)	2.904 (1)	164 (2)
N2—H2*N*···O2	0.87 (1)	1.92 (1)	2.785 (1)	177 (2)
C5—H5*A*···O1^{iii}	0.95	2.56	3.351 (2)	141
C3—H3*A*···*Cg*3^{iv}	0.95	2.66	3.502 (1)	148

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