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2-[6-(4-Chlorophenyl)imidazo[2,1-*b*][1,3]thiazol-2-yl]-*N*′-[(*E*)-4-methoxybenzylidene]acetohydrazide

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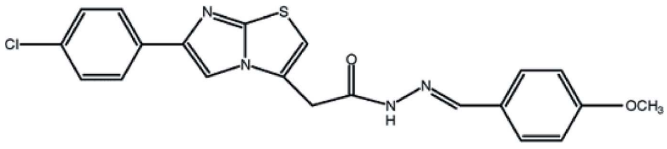
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.007 Å; R factor = 0.059; wR factor = 0.164; data-to-parameter ratio = 12.5.

In the imidazo[2,1-*b*][1,3]thiazole group of the title compound, $C_{21}H_{17}ClN_4O_2S$, the dihedral angle between the thiazole and imidazole rings is 1.9 (2)°. The mean plane of this group makes dihedral angles of 5.5 (2) and 39.9 (2)° with the benzene rings of the chlorophenyl and methoxyphenyl groups, respectively. The dihedral angle between these two benzene rings is 34.4 (2)°. In the crystal, molecules are connected to each other by intermolecular N—H···O hydrogen bonds along the *b* axis, generating a $C(4)$ chain. Weak C—H···π interactions also occur.

Related literature

For the biological activity of imidazo[2,1-*b*][1,3]thiazole derivatives, see: Andreani *et al.* (2005); Barradas *et al.* (2008); Hanson *et al.* (1991); Juspin *et al.* (2010); Shilcrat *et al.* (1991). For details of the synthesis, see: Gürsoy & Ulusoy Güzeldemirci (2007); Ulusoy Güzeldemirci & Küçükbasmacı (2010). For related structures, see: Akkurt *et al.* (2007, 2008). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{17}ClN_4O_2S$
M_r = 424.91
Orthorhombic, $Pca2_1$
a = 13.4591 (6) Å
b = 4.7834 (3) Å
c = 30.4674 (14) Å
V = 1961.50 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 296 K
0.38 × 0.26 × 0.13 mm

Data collection

Stoe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.890, T_{max} = 0.961
10765 measured reflections
3304 independent reflections
2754 reflections with $I > 2\sigma(I)$
R_{int} = 0.092

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.164
S = 1.01
3304 reflections
265 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1611 Friedel pairs
Flack parameter: 0.15 (11)

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

*Cg*1 is the centroid of the N1/N2/C7–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*A*···O1^{i}	0.86	2.08	2.835 (4)	146
C12—H12*A*···*Cg*1^{i}	0.97	2.54	3.282 (5)	133

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2066).

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supporting information

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2-[6-(4-Chlorophenyl)imidazo[2,1-*b*][1,3]thiazol-2-yl]-*N*′-[(*E*)-4-methoxybenzylidene]acetohydrazide

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S1. Comment

Imidazo[2,1-*b*][1,3]thiazole derivatives have demonstrated a broad range of biological activities, including immunomodulatory (Hanson *et al.*, 1991), antibacterial (Juspin *et al.*, 2010), antiviral (Barradas, *et al.*., 2008), antitumoral (Andreani *et al.*, 2005) and antiinflammatory (Shilcrat *et al.*, 1991).

As part of our on-going research aiming on the synthesis of imidazo[2,1-*b*]thiazoles (Gürsoy & Ulusoy Güzeldemirci, 2007; Ulusoy Güzeldemirci & Küçükbasmacı, 2010) and their crystal structures (Akkurt *et al.*, 2007, 2008), we report here the crystal structure of the title compound (I).

In the title molecule of (I), (Fig. 1), the bond lengths and bond angles are normal (Allen *et al.*, 1987). The imidazo[2,1-*b*][1,3]thiazole group is essantially planar with a dihedral angle of 1.9 (2) ° between the thiazole and imidazole rings makes a dihedral angle of 2.99 (15)°.

The mean plane of the imidazo[2,1-*b*][1,3]thiazole group makes dihedral angles of 5.5 (2) and 39.9 (2) ° with the benzene rings of the chlorophenyl and methoxyphenyl groups, respectively. The dihedral angle between these two phenyl rings is 34.4 (2) °.

Molecules are connected to each other by intermolecular N—H···O hydrogen bonds along the *b* axis, generating a C(4) chain (Table 1, Fig. 2). In the crystal structure, a weak C—H···π interaction occurs.

S2. Experimental

[6-(4-Chlorophenyl)imidazo[2,1-*b*]thiazol-3-yl]acetic acid hydrazide (0.005 mol) and 4-methoxybenzaldehyde (0.005 mol) were heated in 100 ml ethanol for 5 h. The precipitate obtained was purified by washing with hot ethanol. Yield: 88%. *M*.p.: 511.5–512.6 K. IR [*v*, cm^{-1}, KBr]: 3212, 3138 (N—H), 1660 (C=O). Analysis calculated for $C_{21}H_{17}ClN_4O_2S$: C 59.36, H 4.03, N 13.19%. Found: C 59.25, H 3.94, N 13.18%.

S3. Refinement

All H atoms were placed in geometrically idealized positions and refined using a riding model, with N—H = 0.86 Å and C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and U_{iso}(H) = 1.5U_{eq}(C) for methyl H, and U_{iso}(H) =1.2U_{eq}(C,*N*) for all other H atoms.

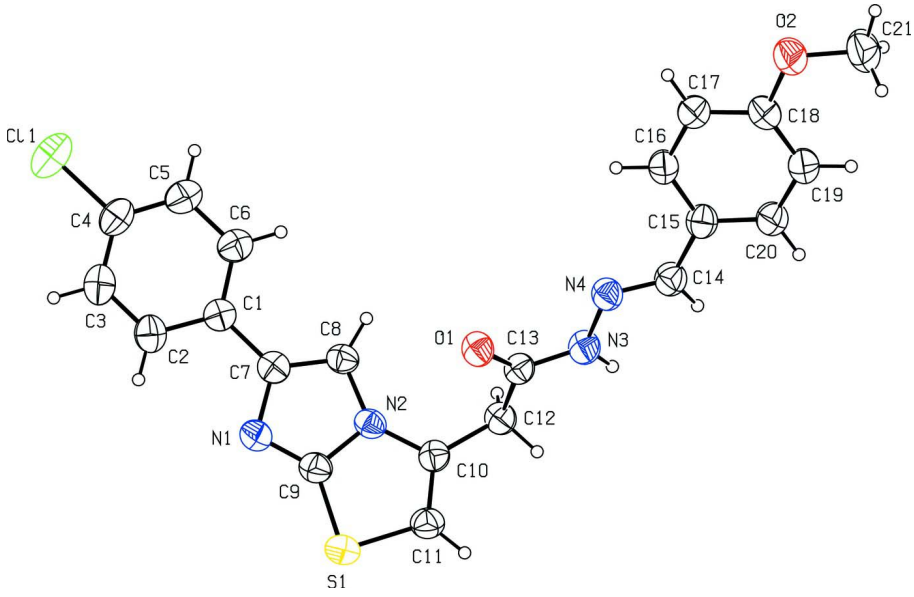

Figure 1

View of the title molecule, with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

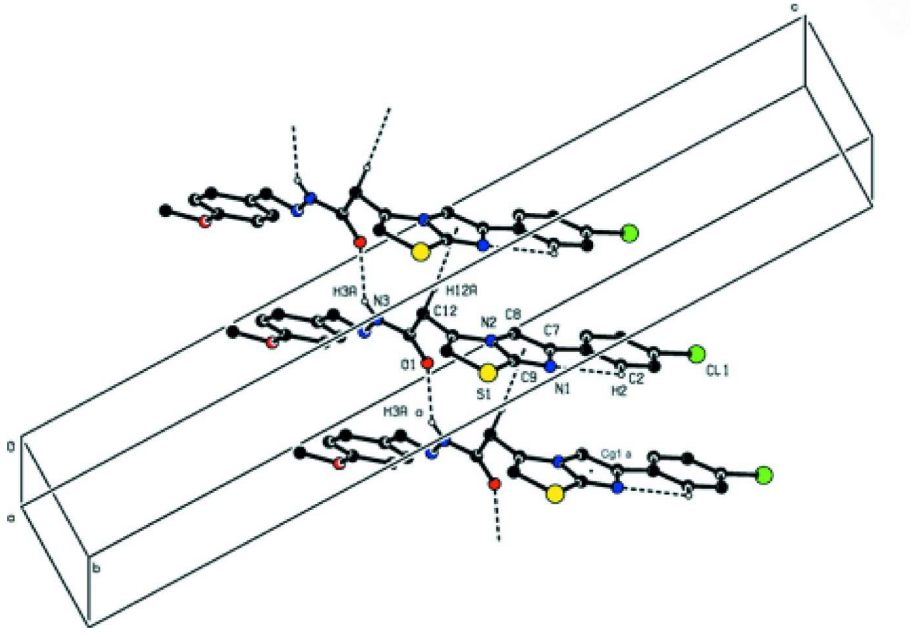

Figure 2

Partial view of the crystal packing showing the N—H···O, C—H···N hydrogen bonding interactions and C—H···π interactions of (I) in the unit cell. All H atoms not involved in hydrogen bonding are omitted for clarity. *Cg*1 is the centroid of ring N1/N2/C7—C9. [Symmetry code: (*a*) x, 1 + y, z].

2-[6-(4-Chlorophenyl)imidazo[2,1-*b*][1,3]thiazol-2-yl]- *N*′-[(*E*)-4-methoxybenzylidene]acetohydrazide

Crystal data

$C_{21}H_{17}ClN_4O_2S$
$M_r = 424.91$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 13.4591\ (6)$ Å
$b = 4.7834\ (3)$ Å
$c = 30.4674\ (14)$ Å
$V = 1961.50\ (18)$ Å^3
$Z = 4$
$F(000) = 880$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15357 reflections
$\theta = 1.3–25.1°$
$\mu = 0.33$ mm^{-1}
$T = 296$ K
Prism, colourless
0.38 × 0.26 × 0.13 mm

Data collection

Stoe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.890$, $T_{max} = 0.961$
10765 measured reflections
3304 independent reflections
2754 reflections with $I > 2\sigma(I)$
$R_{int} = 0.092$
$\theta_{max} = 24.6°$, $\theta_{min} = 1.3°$
$h = -15\rightarrow15$
$k = -5\rightarrow5$
$l = -35\rightarrow35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.164$
$S = 1.01$
3304 reflections
265 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1136P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Extinction coefficient: 0.010 (2)
Absolute structure: Flack (1983), 1611 Friedel pairs
Absolute structure parameter: 0.15 (11)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	0.54087 (14)	1.5430 (3)	0.72891 (5)	0.1113 (6)

S1	1.01901 (8)	0.7353 (3)	0.53219 (5)	0.0824 (4)
O1	0.6911 (2)	0.6101 (5)	0.46534 (10)	0.0706 (10)
O2	0.1795 (3)	0.1793 (9)	0.30456 (13)	0.0947 (12)
N1	0.8812 (3)	0.9668 (8)	0.59159 (12)	0.0709 (11)
N2	0.8350 (2)	0.6242 (7)	0.54579 (11)	0.0612 (10)
N3	0.6651 (3)	0.1742 (7)	0.43926 (12)	0.0689 (11)
N4	0.5793 (3)	0.2476 (7)	0.41650 (13)	0.0676 (11)
C1	0.7215 (3)	1.0549 (9)	0.62971 (14)	0.0647 (12)
C2	0.7662 (4)	1.2522 (10)	0.65723 (15)	0.0770 (14)
C3	0.7105 (4)	1.3995 (11)	0.68731 (17)	0.0863 (19)
C4	0.6104 (4)	1.3556 (10)	0.69031 (16)	0.0800 (19)
C5	0.5640 (4)	1.1665 (12)	0.66394 (17)	0.0823 (17)
C6	0.6196 (4)	1.0159 (11)	0.63367 (15)	0.0767 (17)
C7	0.7810 (3)	0.9024 (9)	0.59711 (15)	0.0653 (12)
C8	0.7513 (3)	0.6957 (8)	0.56975 (14)	0.0630 (12)
C9	0.9110 (3)	0.7939 (9)	0.56040 (15)	0.0680 (12)
C10	0.8635 (3)	0.4461 (8)	0.51164 (14)	0.0620 (12)
C11	0.9596 (3)	0.4809 (10)	0.50111 (17)	0.0720 (17)
C12	0.7937 (3)	0.2362 (8)	0.49197 (16)	0.0655 (14)
C13	0.7124 (3)	0.3618 (8)	0.46392 (14)	0.0596 (11)
C14	0.5417 (4)	0.0495 (10)	0.39367 (16)	0.0723 (16)
C15	0.4478 (4)	0.0818 (9)	0.37059 (15)	0.0700 (14)
C16	0.3780 (4)	0.2839 (9)	0.38208 (16)	0.0730 (16)
C17	0.2884 (4)	0.3090 (11)	0.36042 (17)	0.0790 (17)
C18	0.2698 (4)	0.1353 (10)	0.32490 (17)	0.0750 (16)
C19	0.3377 (4)	−0.0638 (10)	0.31242 (17)	0.0817 (17)
C20	0.4246 (4)	−0.0884 (10)	0.33545 (18)	0.0783 (17)
C21	0.1516 (5)	−0.0120 (16)	0.2706 (2)	0.115 (3)
H2	0.83420	1.28430	0.65520	0.0920*
H3	0.74110	1.52900	0.70560	0.1030*
H3A	0.68770	0.00650	0.43740	0.0830*
H5	0.49580	1.13840	0.66620	0.0980*
H6	0.58800	0.88640	0.61570	0.0920*
H8	0.68810	0.61820	0.56750	0.0760*
H11	0.99130	0.37860	0.47930	0.0860*
H12A	0.76320	0.13000	0.51550	0.0780*
H12B	0.83180	0.10670	0.47420	0.0780*
H14	0.57540	−0.11980	0.39180	0.0870*
H16	0.39220	0.40560	0.40500	0.0880*
H17	0.24140	0.43960	0.36950	0.0950*
H19	0.32490	−0.18020	0.28860	0.0980*
H20	0.46990	−0.22540	0.32710	0.0940*
H21A	0.20130	−0.01150	0.24800	0.1720*
H21B	0.08890	0.04400	0.25840	0.1720*
H21C	0.14580	−0.19670	0.28270	0.1720*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1479 (14)	0.0934 (9)	0.0926 (8)	0.0296 (9)	0.0312 (9)	−0.0020 (8)
S1	0.0569 (5)	0.0919 (8)	0.0983 (8)	−0.0039 (5)	0.0019 (6)	−0.0118 (7)
O1	0.0780 (18)	0.0475 (13)	0.0862 (18)	0.0048 (13)	−0.0115 (16)	0.0021 (14)
O2	0.086 (2)	0.102 (2)	0.096 (2)	0.004 (2)	−0.020 (2)	−0.020 (2)
N1	0.0618 (18)	0.076 (2)	0.075 (2)	0.0001 (17)	−0.0067 (18)	−0.005 (2)
N2	0.0554 (17)	0.0586 (16)	0.0697 (19)	−0.0003 (14)	−0.0055 (15)	0.0055 (15)
N3	0.075 (2)	0.0517 (17)	0.080 (2)	0.0084 (15)	−0.0098 (19)	0.0007 (16)
N4	0.069 (2)	0.0569 (17)	0.077 (2)	0.0017 (15)	−0.0060 (17)	−0.0023 (17)
C1	0.068 (2)	0.063 (2)	0.063 (2)	0.0025 (19)	−0.0017 (18)	0.0064 (18)
C2	0.093 (3)	0.068 (2)	0.070 (2)	−0.006 (2)	−0.004 (2)	0.000 (2)
C3	0.108 (4)	0.077 (3)	0.074 (3)	0.001 (3)	−0.007 (3)	−0.010 (3)
C4	0.099 (4)	0.070 (3)	0.071 (3)	0.017 (2)	0.009 (3)	0.002 (2)
C5	0.079 (3)	0.088 (3)	0.080 (3)	0.015 (3)	0.007 (3)	0.003 (3)
C6	0.074 (3)	0.083 (3)	0.073 (3)	0.006 (2)	0.005 (2)	0.003 (2)
C7	0.067 (2)	0.062 (2)	0.067 (2)	0.0017 (18)	−0.004 (2)	0.007 (2)
C8	0.057 (2)	0.062 (2)	0.070 (2)	−0.0038 (18)	0.0016 (18)	0.0042 (19)
C9	0.060 (2)	0.069 (2)	0.075 (2)	0.0014 (19)	−0.003 (2)	0.003 (2)
C10	0.066 (2)	0.055 (2)	0.065 (2)	0.0055 (17)	−0.0037 (19)	0.0025 (18)
C11	0.062 (3)	0.072 (3)	0.082 (3)	0.0067 (19)	−0.002 (2)	0.000 (2)
C12	0.068 (2)	0.0504 (19)	0.078 (3)	0.0026 (17)	−0.006 (2)	0.0034 (18)
C13	0.066 (2)	0.0478 (18)	0.065 (2)	−0.0003 (16)	0.0044 (19)	0.0037 (17)
C14	0.076 (3)	0.064 (2)	0.077 (3)	0.002 (2)	−0.001 (2)	−0.002 (2)
C15	0.078 (3)	0.061 (2)	0.071 (2)	−0.001 (2)	0.000 (2)	0.000 (2)
C16	0.077 (3)	0.068 (2)	0.074 (3)	−0.002 (2)	−0.005 (2)	−0.012 (2)
C17	0.072 (3)	0.076 (3)	0.089 (3)	0.005 (2)	−0.003 (2)	−0.013 (2)
C18	0.071 (3)	0.080 (3)	0.074 (2)	−0.006 (2)	−0.010 (2)	−0.001 (2)
C19	0.080 (3)	0.081 (3)	0.084 (3)	0.000 (2)	−0.009 (2)	−0.018 (2)
C20	0.074 (3)	0.068 (3)	0.093 (3)	0.005 (2)	−0.005 (2)	−0.013 (2)
C21	0.113 (5)	0.123 (5)	0.108 (4)	0.001 (4)	−0.034 (4)	−0.034 (4)

Geometric parameters (Å, º)

Cl1—C4	1.750 (5)	C12—C13	1.513 (6)
S1—C9	1.712 (4)	C14—C15	1.455 (7)
S1—C11	1.737 (5)	C15—C20	1.381 (7)
O1—C13	1.223 (5)	C15—C16	1.393 (7)
O2—C18	1.380 (7)	C16—C17	1.380 (7)
O2—C21	1.431 (8)	C17—C18	1.387 (7)
N1—C7	1.394 (6)	C18—C19	1.374 (7)
N1—C9	1.322 (6)	C19—C20	1.369 (8)
N2—C8	1.385 (5)	C2—H2	0.9300
N2—C9	1.380 (5)	C3—H3	0.9300
N2—C10	1.398 (5)	C5—H5	0.9300
N3—N4	1.392 (6)	C6—H6	0.9300
N3—C13	1.332 (5)	C8—H8	0.9300

N4—C14	1.280 (6)	C11—H11	0.9300
N3—H3A	0.8600	C12—H12A	0.9700
C1—C6	1.389 (7)	C12—H12B	0.9700
C1—C7	1.470 (6)	C14—H14	0.9300
C1—C2	1.399 (6)	C16—H16	0.9300
C2—C3	1.378 (7)	C17—H17	0.9300
C3—C4	1.367 (8)	C19—H19	0.9300
C4—C5	1.362 (7)	C20—H20	0.9300
C5—C6	1.389 (7)	C21—H21A	0.9600
C7—C8	1.354 (6)	C21—H21B	0.9600
C10—C12	1.500 (6)	C21—H21C	0.9600
C10—C11	1.343 (6)		

C9—S1—C11	89.9 (2)	C16—C17—C18	118.6 (5)
C18—O2—C21	117.3 (5)	O2—C18—C19	124.6 (5)
C7—N1—C9	104.0 (4)	O2—C18—C17	114.7 (5)
C8—N2—C9	106.7 (3)	C17—C18—C19	120.7 (5)
C8—N2—C10	140.0 (3)	C18—C19—C20	119.1 (5)
C9—N2—C10	113.3 (3)	C15—C20—C19	122.7 (5)
N4—N3—C13	120.5 (3)	C1—C2—H2	120.00
N3—N4—C14	114.3 (4)	C3—C2—H2	120.00
C13—N3—H3A	120.00	C2—C3—H3	120.00
N4—N3—H3A	120.00	C4—C3—H3	120.00
C2—C1—C7	120.4 (4)	C4—C5—H5	120.00
C2—C1—C6	117.6 (4)	C6—C5—H5	120.00
C6—C1—C7	122.0 (4)	C1—C6—H6	119.00
C1—C2—C3	120.7 (5)	C5—C6—H6	119.00
C2—C3—C4	120.2 (5)	N2—C8—H8	127.00
C3—C4—C5	121.0 (5)	C7—C8—H8	127.00
Cl1—C4—C5	119.5 (4)	S1—C11—H11	123.00
Cl1—C4—C3	119.6 (4)	C10—C11—H11	123.00
C4—C5—C6	119.3 (5)	C10—C12—H12A	109.00
C1—C6—C5	121.3 (5)	C10—C12—H12B	109.00
N1—C7—C1	120.0 (4)	C13—C12—H12A	109.00
N1—C7—C8	111.9 (4)	C13—C12—H12B	109.00
C1—C7—C8	128.2 (4)	H12A—C12—H12B	108.00
N2—C8—C7	105.4 (3)	N4—C14—H14	119.00
N1—C9—N2	112.0 (4)	C15—C14—H14	119.00
S1—C9—N1	136.1 (3)	C15—C16—H16	119.00
S1—C9—N2	111.8 (3)	C17—C16—H16	119.00
N2—C10—C11	111.5 (4)	C16—C17—H17	121.00
N2—C10—C12	122.2 (3)	C18—C17—H17	121.00
C11—C10—C12	126.2 (4)	C18—C19—H19	120.00
S1—C11—C10	113.6 (4)	C20—C19—H19	120.00
C10—C12—C13	114.4 (3)	C15—C20—H20	119.00
N3—C13—C12	113.4 (3)	C19—C20—H20	119.00
O1—C13—C12	122.4 (4)	O2—C21—H21A	110.00
O1—C13—N3	124.2 (4)	O2—C21—H21B	109.00

N4—C14—C15	121.9 (4)	O2—C21—H21C	109.00
C16—C15—C20	116.9 (5)	H21A—C21—H21B	110.00
C14—C15—C16	122.6 (4)	H21A—C21—H21C	110.00
C14—C15—C20	120.6 (4)	H21B—C21—H21C	109.00
C15—C16—C17	122.0 (4)		

C11—S1—C9—N2	−0.2 (3)	C6—C1—C7—C8	−5.7 (7)
C11—S1—C9—N1	−177.4 (5)	C2—C1—C7—C8	176.1 (4)
C9—S1—C11—C10	0.4 (4)	C1—C2—C3—C4	−0.5 (7)
C21—O2—C18—C17	−173.8 (5)	C2—C3—C4—Cl1	179.6 (4)
C21—O2—C18—C19	5.6 (8)	C2—C3—C4—C5	0.2 (8)
C7—N1—C9—N2	0.2 (5)	Cl1—C4—C5—C6	−179.3 (4)
C7—N1—C9—S1	177.4 (4)	C3—C4—C5—C6	0.2 (8)
C9—N1—C7—C1	−180.0 (4)	C4—C5—C6—C1	−0.2 (8)
C9—N1—C7—C8	−0.1 (5)	C1—C7—C8—N2	179.9 (4)
C9—N2—C8—C7	0.1 (4)	N1—C7—C8—N2	0.0 (5)
C10—N2—C9—N1	177.8 (4)	C11—C10—C12—C13	−111.4 (5)
C10—N2—C8—C7	−177.0 (5)	N2—C10—C11—S1	−0.6 (5)
C8—N2—C9—S1	−178.1 (3)	C12—C10—C11—S1	−177.6 (3)
C9—N2—C10—C12	177.6 (4)	N2—C10—C12—C13	71.8 (5)
C10—N2—C9—S1	−0.1 (4)	C10—C12—C13—O1	−16.2 (6)
C8—N2—C9—N1	−0.2 (5)	C10—C12—C13—N3	166.1 (4)
C8—N2—C10—C12	−5.4 (7)	N4—C14—C15—C20	158.2 (5)
C9—N2—C10—C11	0.4 (5)	N4—C14—C15—C16	−21.1 (7)
C8—N2—C10—C11	177.4 (5)	C14—C15—C20—C19	−179.3 (5)
N4—N3—C13—O1	−7.0 (7)	C16—C15—C20—C19	0.1 (7)
C13—N3—N4—C14	179.3 (4)	C14—C15—C16—C17	−178.8 (5)
N4—N3—C13—C12	170.6 (4)	C20—C15—C16—C17	1.9 (7)
N3—N4—C14—C15	175.0 (4)	C15—C16—C17—C18	−3.0 (8)
C2—C1—C7—N1	−4.1 (6)	C16—C17—C18—C19	2.1 (8)
C2—C1—C6—C5	−0.2 (7)	C16—C17—C18—O2	−178.5 (4)
C6—C1—C2—C3	0.5 (7)	O2—C18—C19—C20	−179.6 (5)
C7—C1—C6—C5	−178.4 (5)	C17—C18—C19—C20	−0.2 (8)
C7—C1—C2—C3	178.8 (4)	C18—C19—C20—C15	−0.9 (8)
C6—C1—C7—N1	174.1 (4)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the N1/N2/C7–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{i}	0.86	2.08	2.835 (4)	146
C2—H2···N1	0.93	2.54	2.874 (6)	101
C12—H12*A*···*Cg*1^{i}	0.97	2.54	3.282 (5)	133

Symmetry code: (i) *x*, *y*−1, *z*.