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2-Benzoylamino-*N*-[5-(4-bromophenyl)-1,3,4-thiadiazol-2-yl]ethanamide

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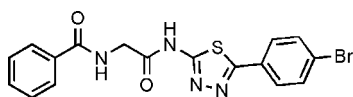
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.109; wR factor = 0.281; data-to-parameter ratio = 11.4.

In the structure of the title compound, $\text{C}_{17}\text{H}_{13}\text{BrN}_4\text{O}_2\text{S}$, the dihedral angle between the two benzene rings is 38.5 (1°); the angle between the 4-bromobenzene and thiadiazole rings is 1.3 (1°). The conformations of the $\text{N}-\text{H}$ and $\text{C}=\text{O}$ bonds are *anti* with respect to each other. The structure displays intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding, with both interactions leading to inversion dimers.

Related literature

For 1,3,4-thiadiazole scaffold compounds and their biological activity, see: Tu *et al.* (2008). For the synthesis, see: Foroumadi *et al.* (1999); Levy & Palmer (1942); Song *et al.* (1992). For related structures, see: Gowda *et al.* (2008); Li, Huang *et al.* (2008); Li, Li *et al.* (2008).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{13}\text{BrN}_4\text{O}_2\text{S}$
 $M_r = 417.28$
Triclinic, $P\bar{1}$
 $a = 4.020$ (4) Å
 $b = 13.706$ (9) Å
 $c = 16.210$ (5) Å
 $\alpha = 113.334$ (17°)
 $\beta = 94.018$ (19°)

$\gamma = 92.78$ (2°)
 $V = 815.2$ (10) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 2.67$ mm⁻¹
 $T = 298$ (2) K
 $0.54 \times 0.17 \times 0.04$ mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2008)
 $T_{\text{min}} = 0.591$, $T_{\text{max}} = 0.914$
4633 measured reflections
2592 independent reflections
1097 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.109$
 $wR(F^2) = 0.281$
 $S = 0.82$
2592 reflections
227 parameters
6 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.40$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C16}-\text{H16A}\cdots\text{O2}^{\text{i}}$	0.93	2.49	3.400 (5)	168
$\text{N2}-\text{H2A}\cdots\text{O1}^{\text{ii}}$	0.86	1.99	2.835 (5)	167

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *APEX2* (Bruker, 2004); software used to prepare material for publication: *APEX2* (Bruker, 2004) and *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2304).

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supporting information

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2-Benzoylamino-*N*-[5-(4-bromophenyl)-1,3,4-thiadiazol-2-yl]ethanamide

Hui-Ming Huang, Shi-Yuan Luo, Shao-Hua Li, Cheng-Mei Liu and Guo-Gang Tu

S1. Comment

In our previous work, 1,3,4-thiadiazole scaffold compounds and their biological activity have been studied (Tu *et al.*, 2008). In view of the importance of these organic materials, the title compound (Fig. 1) was synthesized (Foroumadi *et al.*, 1999; Levy & Palmer 1942; Song *et al.*, 1992) and its crystal structure is reported here.

In the structure of the title compound, C₁₇H₁₃BrN₄O₂S, the dihedral angle between the *p*-bromobenzene and thiadiazole rings is 1.3 (1)°; the angle between the two benzene rings is 38.5 (1)°. The conformations of the N—H and C=O bonds are *anti* with respect to each other. Bond lengths and angles are in normal ranges and comparable to those in related structures (Gowda *et al.*, 2008; Li, Huang *et al.*, 2008; Li, Li *et al.*, 2008). In the crystal structure, molecules are linked through intermolecular C—H⋯O and N—H⋯O hydrogen bonds, forming a three-dimensional network (Table 1, Figure 2).

S2. Experimental

N,N-Dicyclohexylcarbodiimide (5.7 mmol) was added to a cooled solution of *N*-benzoylglycine (5.6 mmol) and *N*-hydroxysuccinimide (5.6 mmol) in freshly distilled dioxane (30 ml). The reaction mixture was stirred overnight at room temperature. The insoluble material was filtered off and washed with cold dioxane. 2-Amino-5-(4-bromophenyl)-1,3,4-thiadiazole (5.5 mmol) was added to the filtrate and the reaction mixture was stirred for 48 h at room temperature. The solvent was removed under reduced pressure. The residue was dissolved in EtOAc and the insoluble material was filtered off. The filtrate was washed successively with saturated Na₂CO₃ solution (20 ml, *x* 3), water (20 ml, *x* 1), 0.1 M HCl (20 ml, *x* 3) and water (20 ml, *x* 1). The organic layer evaporated *in vacuo*, and the residue was recrystallized from methanol. Colorless block-shaped single crystals of the title compound suitable for X-ray diffraction analysis precipitated after several days. Yield: 37.0%; mp: 271–273°C.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model; Csp²—H = 0.93 Å, Csp³—H = 0.97 Å and N—H = 0.86 Å; *U*_{iso}(H) = 1.2 *U*_{eq}(C,N). We made several attempts to obtain better quality data for this structure. However, due to poor crystal quality and possible disorder, the *R* and *wR* values are high. The maximum residual electron density occurs 1.23 Å from atom Br1, and the minimum residual electron density is located 1.29 Å from atom Br1.

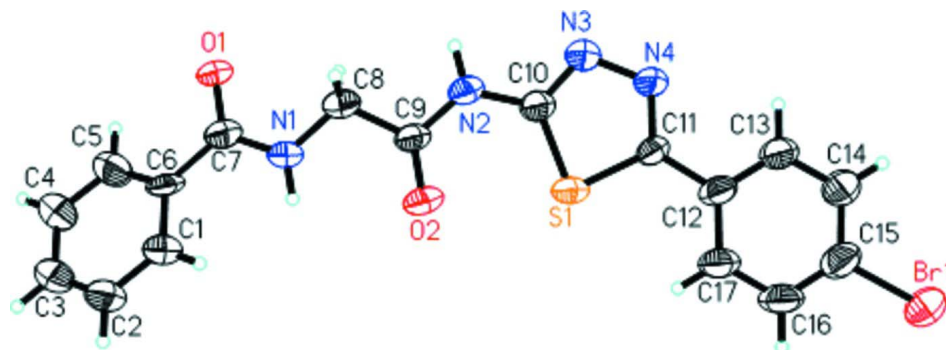


Figure 1

Molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

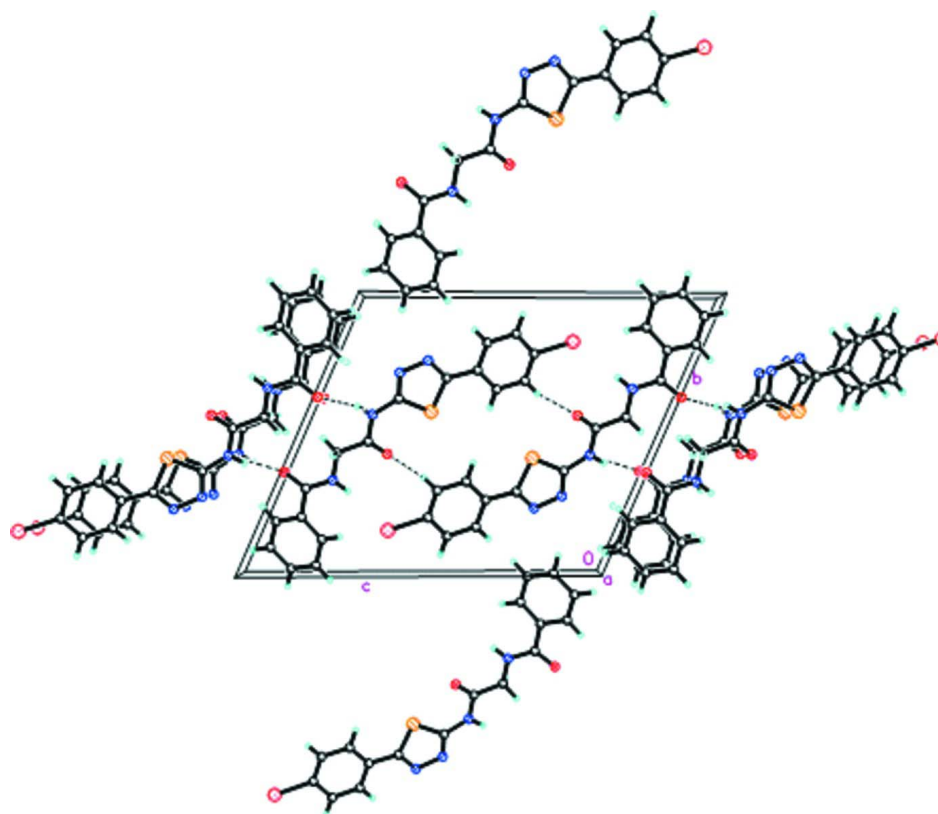


Figure 2

The crystal packing of the title compound, viewed along the *a* axis with hydrogen bonds drawn as dashed lines.

2-Benzoylamino-*N*-[5-(4-bromophenyl)-1,3,4-thiadiazol-2-yl]ethanamide

Crystal data

$C_{17}H_{13}BrN_4O_2S$

$M_r = 417.28$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 4.020\ (4)\ \text{\AA}$

$b = 13.706\ (9)\ \text{\AA}$

$c = 16.210\ (5)\ \text{\AA}$

$\alpha = 113.334\ (17)^\circ$

$\beta = 94.018\ (19)^\circ$

$\gamma = 92.78\ (2)^\circ$

$V = 815.2 (10) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 420.0$
 $D_x = 1.700 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 1179 reflections

$\theta = 2.6\text{--}23.7^\circ$
 $\mu = 2.67 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block, colourless
 $0.54 \times 0.17 \times 0.04 \text{ mm}$

Data collection

Bruker X8 APEXII
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
 $T_{\min} = 0.591, T_{\max} = 0.914$

4633 measured reflections
 2592 independent reflections
 1097 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$
 $\theta_{\max} = 25.0^\circ, \theta_{\min} = 2.5^\circ$
 $h = -4 \rightarrow 4$
 $k = -16 \rightarrow 16$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.109$
 $wR(F^2) = 0.281$
 $S = 0.82$
 2592 reflections
 227 parameters
 6 restraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.1951P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.019$
 $\Delta\rho_{\max} = 1.67 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -1.40 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97 (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.022 (2)

Special details

Experimental. $^1\text{H-NMR}$ (DMSO- d_6): δ 4.24–4.25(d, $J=5.08 \text{ Hz}$, 2H), 7.49–7.57 (m, 3H), 7.73–7.75 (d, $J=8.04 \text{ Hz}$, 2H), 7.89–7.91(t, $J=3.60 \text{ Hz}$, 4H), 9.01 (s, 1H), 12.91 (s, 1H). ESI-MS: m/z $[M+H]^+$ 417.3.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.19570 (14)	0.16142 (4)	0.64242 (3)	0.07526 (19)
S1	0.3284 (3)	0.41677 (8)	0.33059 (7)	0.0550 (4)
O1	0.2257 (8)	0.6333 (2)	-0.00717 (17)	0.0636 (9)
O2	0.2253 (9)	0.5689 (2)	0.25867 (18)	0.0687 (8)
N1	0.2711 (9)	0.6635 (2)	0.1388 (2)	0.0551 (12)
H1A	0.2352	0.7034	0.1931	0.066*
N3	0.5949 (10)	0.2787 (3)	0.1998 (2)	0.0621 (13)

N4	0.5645 (10)	0.2351 (2)	0.2632 (2)	0.0597 (8)
N2	0.4834 (9)	0.4276 (2)	0.1728 (2)	0.0539 (8)
H2A	0.5726	0.3992	0.1229	0.065*
C4	-0.2078 (13)	0.9136 (3)	0.0368 (3)	0.0711 (18)
H4B	-0.3108	0.9254	-0.0112	0.085*
C5	-0.0907 (12)	0.8176 (3)	0.0241 (3)	0.0610 (16)
H5A	-0.1231	0.7628	-0.0332	0.073*
C10	0.4756 (11)	0.3703 (3)	0.2263 (3)	0.0512 (11)
C16	0.1797 (12)	0.3039 (3)	0.5556 (3)	0.0632 (17)
H16A	0.0838	0.3486	0.6061	0.076*
C15	0.2691 (13)	0.2067 (3)	0.5481 (3)	0.0603 (10)
C12	0.3711 (10)	0.2674 (3)	0.4098 (2)	0.0471 (9)
C14	0.4058 (11)	0.1370 (3)	0.4729 (3)	0.0598 (11)
H14A	0.4596	0.0701	0.4688	0.072*
C17	0.2354 (12)	0.3345 (3)	0.4857 (3)	0.0587 (11)
H17A	0.1807	0.4014	0.4900	0.070*
C8	0.4114 (12)	0.5638 (3)	0.1200 (3)	0.0560 (15)
H8A	0.6486	0.5723	0.1144	0.067*
H8B	0.3068	0.5116	0.0627	0.067*
C9	0.3647 (11)	0.5237 (3)	0.1913 (2)	0.0475 (10)
C11	0.4297 (11)	0.2963 (3)	0.3341 (2)	0.0483 (10)
C13	0.4598 (12)	0.1698 (3)	0.4041 (3)	0.0601 (16)
H13A	0.5571	0.1253	0.3537	0.072*
C7	0.1970 (11)	0.6938 (3)	0.0722 (3)	0.0521 (13)
C6	0.0730 (11)	0.7991 (3)	0.0926 (2)	0.0489 (14)
C2	-0.0154 (12)	0.9776 (3)	0.1919 (3)	0.0601 (16)
H2B	0.0074	1.0320	0.2494	0.072*
C3	-0.1698 (12)	0.9930 (3)	0.1230 (3)	0.0643 (17)
H3B	-0.2533	1.0585	0.1332	0.077*
C1	0.1113 (12)	0.8805 (3)	0.1780 (3)	0.0555 (15)
H1B	0.2216	0.8701	0.2259	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0941 (4)	0.0888 (3)	0.0604 (2)	0.0226 (3)	0.0361 (2)	0.04206 (19)
S1	0.0804 (8)	0.0441 (5)	0.0406 (5)	0.0193 (5)	0.0286 (5)	0.0118 (4)
O1	0.106 (2)	0.0501 (14)	0.0414 (6)	0.0279 (14)	0.0433 (10)	0.0174 (7)
O2	0.1043 (12)	0.0616 (16)	0.0469 (7)	0.0256 (13)	0.0439 (6)	0.0207 (9)
N1	0.082 (3)	0.0452 (17)	0.0435 (16)	0.0255 (16)	0.0332 (18)	0.0165 (13)
N3	0.099 (3)	0.0488 (17)	0.0448 (17)	0.0288 (18)	0.0270 (19)	0.0193 (13)
N4	0.1059 (15)	0.0386 (15)	0.0399 (8)	0.0252 (12)	0.0297 (7)	0.0154 (8)
N2	0.075 (2)	0.0474 (5)	0.0474 (5)	0.0157 (15)	0.0353 (16)	0.0212 (3)
C4	0.097 (4)	0.049 (2)	0.070 (3)	0.025 (2)	0.022 (3)	0.022 (2)
C5	0.080 (3)	0.042 (2)	0.053 (2)	0.012 (2)	0.009 (2)	0.0102 (18)
C10	0.073 (3)	0.0390 (7)	0.0442 (7)	0.0091 (19)	0.024 (2)	0.0156 (4)
C16	0.080 (3)	0.054 (2)	0.051 (2)	0.012 (2)	0.034 (2)	0.0102 (19)
C15	0.0825 (16)	0.0564 (19)	0.0442 (9)	-0.0018 (12)	0.0194 (8)	0.0211 (8)

C12	0.0546 (15)	0.0498 (18)	0.0351 (9)	0.0036 (12)	0.0172 (7)	0.0131 (8)
C14	0.066 (2)	0.066 (2)	0.0600 (12)	0.0136 (14)	0.0282 (10)	0.0337 (10)
C17	0.078 (2)	0.050 (2)	0.0448 (11)	0.0131 (15)	0.0261 (10)	0.0109 (10)
C8	0.064 (3)	0.061 (2)	0.053 (2)	0.026 (2)	0.035 (2)	0.0269 (16)
C9	0.0644 (16)	0.041 (2)	0.0353 (8)	0.0082 (16)	0.0210 (7)	0.0104 (12)
C11	0.0753 (18)	0.0407 (18)	0.0336 (10)	0.0106 (14)	0.0223 (9)	0.0165 (9)
C13	0.094 (3)	0.042 (2)	0.046 (2)	0.010 (2)	0.030 (2)	0.0159 (16)
C7	0.071 (3)	0.047 (2)	0.0344 (7)	0.0104 (19)	0.0185 (14)	0.0105 (9)
C6	0.061 (3)	0.047 (2)	0.0339 (18)	0.0118 (19)	0.030 (2)	0.0067 (16)
C2	0.078 (3)	0.043 (2)	0.050 (2)	0.009 (2)	0.019 (2)	0.0062 (18)
C3	0.080 (3)	0.052 (2)	0.065 (3)	0.031 (2)	0.025 (3)	0.0211 (19)
C1	0.071 (3)	0.047 (2)	0.046 (2)	0.016 (2)	0.023 (2)	0.0120 (17)

Geometric parameters (Å, °)

Br1—C15	1.898 (5)	C16—C17	1.382 (7)
S1—C10	1.714 (4)	C16—H16A	0.9300
S1—C11	1.741 (5)	C15—C14	1.387 (6)
O1—C7	1.242 (4)	C12—C13	1.370 (6)
O2—C9	1.214 (5)	C12—C17	1.380 (5)
N1—C7	1.323 (6)	C12—C11	1.461 (6)
N1—C8	1.430 (5)	C14—C13	1.383 (7)
N1—H1A	0.8600	C14—H14A	0.9300
N3—C10	1.285 (5)	C17—H17A	0.9300
N3—N4	1.387 (6)	C8—C9	1.483 (7)
N4—C11	1.299 (5)	C8—H8A	0.9700
N2—C9	1.349 (5)	C8—H8B	0.9700
N2—C10	1.381 (6)	C13—H13A	0.9300
N2—H2A	0.8600	C7—C6	1.469 (6)
C4—C5	1.361 (7)	C6—C1	1.383 (5)
C4—C3	1.382 (6)	C2—C3	1.335 (7)
C4—H4B	0.9300	C2—C1	1.388 (6)
C5—C6	1.367 (7)	C2—H2B	0.9300
C5—H5A	0.9300	C3—H3B	0.9300
C16—C15	1.359 (7)	C1—H1B	0.9300
C10—S1—C11	86.0 (2)	C16—C17—H17A	119.5
C7—N1—C8	119.6 (3)	N1—C8—C9	112.3 (3)
C7—N1—H1A	120.2	N1—C8—H8A	109.1
C8—N1—H1A	120.2	C9—C8—H8A	109.1
C10—N3—N4	110.7 (4)	N1—C8—H8B	109.1
C11—N4—N3	113.3 (3)	C9—C8—H8B	109.1
C9—N2—C10	126.3 (3)	H8A—C8—H8B	107.9
C9—N2—H2A	116.8	O2—C9—N2	121.9 (4)
C10—N2—H2A	116.8	O2—C9—C8	125.0 (4)
C5—C4—C3	118.3 (5)	N2—C9—C8	113.1 (3)
C5—C4—H4B	120.9	N4—C11—C12	123.3 (4)
C3—C4—H4B	120.9	N4—C11—S1	113.4 (3)

C4—C5—C6	122.2 (4)	C12—C11—S1	123.3 (3)
C4—C5—H5A	118.9	C12—C13—C14	120.4 (4)
C6—C5—H5A	118.9	C12—C13—H13A	119.8
N3—C10—N2	119.8 (4)	C14—C13—H13A	119.8
N3—C10—S1	116.5 (4)	O1—C7—N1	120.5 (4)
N2—C10—S1	123.6 (3)	O1—C7—C6	120.0 (4)
C15—C16—C17	118.0 (4)	N1—C7—C6	119.4 (3)
C15—C16—H16A	121.0	C5—C6—C1	118.3 (4)
C17—C16—H16A	121.0	C5—C6—C7	118.5 (3)
C16—C15—C14	122.6 (5)	C1—C6—C7	123.2 (4)
C16—C15—Br1	119.4 (3)	C3—C2—C1	120.2 (4)
C14—C15—Br1	118.0 (4)	C3—C2—H2B	119.9
C13—C12—C17	119.7 (4)	C1—C2—H2B	119.9
C13—C12—C11	117.6 (3)	C2—C3—C4	121.2 (4)
C17—C12—C11	122.6 (4)	C2—C3—H3B	119.4
C13—C14—C15	118.2 (4)	C4—C3—H3B	119.4
C13—C14—H14A	120.9	C6—C1—C2	119.8 (4)
C15—C14—H14A	120.9	C6—C1—H1B	120.1
C12—C17—C16	121.0 (4)	C2—C1—H1B	120.1
C12—C17—H17A	119.5		
C10—N3—N4—C11	-1.0 (5)	C13—C12—C11—N4	-0.9 (6)
C3—C4—C5—C6	-2.5 (8)	C17—C12—C11—N4	178.3 (4)
N4—N3—C10—N2	179.7 (4)	C13—C12—C11—S1	179.6 (3)
N4—N3—C10—S1	2.2 (5)	C17—C12—C11—S1	-1.2 (6)
C9—N2—C10—N3	179.2 (4)	C10—S1—C11—N4	1.5 (3)
C9—N2—C10—S1	-3.6 (6)	C10—S1—C11—C12	-178.9 (4)
C11—S1—C10—N3	-2.2 (4)	C17—C12—C13—C14	1.8 (6)
C11—S1—C10—N2	-179.5 (4)	C11—C12—C13—C14	-179.0 (4)
C17—C16—C15—C14	-1.5 (7)	C15—C14—C13—C12	-1.8 (7)
C17—C16—C15—Br1	-179.8 (3)	C8—N1—C7—O1	5.2 (6)
C16—C15—C14—C13	1.7 (7)	C8—N1—C7—C6	-176.1 (4)
Br1—C15—C14—C13	-179.9 (3)	C4—C5—C6—C1	1.8 (7)
C13—C12—C17—C16	-1.6 (6)	C4—C5—C6—C7	-178.7 (5)
C11—C12—C17—C16	179.2 (4)	O1—C7—C6—C5	17.2 (7)
C15—C16—C17—C12	1.4 (7)	N1—C7—C6—C5	-161.5 (4)
C7—N1—C8—C9	-159.0 (4)	O1—C7—C6—C1	-163.3 (4)
C10—N2—C9—O2	-2.3 (6)	N1—C7—C6—C1	18.0 (7)
C10—N2—C9—C8	-180.0 (4)	C1—C2—C3—C4	0.1 (8)
N1—C8—C9—O2	-0.2 (6)	C5—C4—C3—C2	1.6 (8)
N1—C8—C9—N2	177.4 (3)	C5—C6—C1—C2	0.0 (7)
N3—N4—C11—C12	179.8 (4)	C7—C6—C1—C2	-179.5 (4)
N3—N4—C11—S1	-0.6 (5)	C3—C2—C1—C6	-0.9 (8)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C16—H16A...O2 ⁱ	0.93	2.49	3.400 (5)	168

N2—H2A···O1 ⁱⁱ	0.86	1.99	2.835 (5)	167
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Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x+1, -y+1, -z$.