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1-[2-(2,4-Dinitrobenzylideneamino)-phenyl]-3-phenylthiourea

M. Umadevi,[a] S. Devaraj,[b] M. Kandaswamy,[b] G. Chakkaravarthi[c] and V. Manivannan[d]*

[a]Department of Chemistry, Pallavan College of Engineering, Kanchipuram 631 502, Tamilnadu, India, [b]Deparment of Inorganic Chemistry, School of Chemical Sceinces, University of Madras, Guindy Campus, Chennai 600 025, India, [c]Department of Physics, CPCL Polytechnic College, Chennai 600 068, India, and [d]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamilnadu, India
Correspondence e-mail: manivan_1999@yahoo.com

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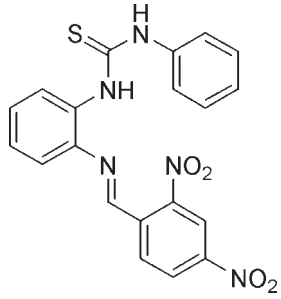
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.137; data-to-parameter ratio = 25.4.

In the title compound, $C_{20}H_{15}N_5O_4S$, the central benzene ring makes dihedral angles of 59.5 (1) and 51.7 (1)°, respectively, with the terminal phenyl and benzene rings. The molecular structure exhibits weak intramolecular N—H···N and C—H···S interactions. In the crystal structure, molecules are linked by weak intermolecular N—H···S and C—H···O interactions, forming a chain along [1$\bar{1}$1].

Related literature

For the biological activity of thioureas, see: Huebner *et al.* (1953); Madan & Taneja (1991); Manjula *et al.* (2009). For related structures, see: Gayathri *et al.* (2007, 2008). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{20}H_{15}N_5O_4S$
M_r = 421.43
Monoclinic, $P2_1/c$
a = 8.362 (5) Å
b = 18.767 (3) Å
c = 12.379 (4) Å
β = 94.827 (5)°
V = 1935.7 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 295 K
0.20 × 0.16 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.968
28336 measured reflections
6878 independent reflections
4509 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.137
S = 1.02
6878 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 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
N4—H4A···N3	0.86	2.14	2.614 (2)	114
C3—H3···S1	0.93	2.55	3.215 (2)	128
N4—H4A···N3	0.86	2.14	2.614 (2)	114
N5—H5A···S1^{i}	0.86	2.49	3.284 (2)	155
C12—H12···O3^{ii}	0.93	2.57	3.397 (3)	148

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

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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors wish to acknowledge IIT, Madras for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2457).

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supporting information

Acta Cryst. (2009). E**65**, o2447 [doi:10.1107/S1600536809035880]

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M. Umadevi, S. Devaraj, M. Kandaswamy, G. Chakkaravarthi and V. Manivannan

S1. Comment

Thioureas are known to exhibit antiviral, antibacterial, anticancer (Madan & Taneja, 1991; Manjula *et al.*, 2009), antifungal, antitubercular, antithyroidal, herbicidal and insecticidal (Huebner *et al.*, 1953) activities.

The geometric parameters in (I), (Fig. 1) agree with the reported values of similar structures (Gayathri *et al.*, 2007, 2008). The benzene ring C1—C6 makes the dihedral angle of 59.5 (1)° with the phenyl ring C15—C20 and 51.7 (1)° with the dinitrobenzene ring C8—C13.

The molecular structure of (I) exhibits weak intramolecular N—H···N, C—H···S and C—H···O interactions and the crystal structure is stabilized by weak intermolecular N—H···S and C—H···O interactions (Table 1 and Fig. 2). The intermolecular N5—H5A···S1 interaction generates an eight-membered ring, with graph-set motif $R_2^2(8)$ and the C12—H12···O3 interaction generates a ten-membered ring, with graph-set motif $R_2^2(10)$ (Bernstein, 1995).

S2. Experimental

To the solution of 1-(2-aminophenyl)-3-phenylthiourea (0.3 g, 1.2 mmol) in methanol (25 ml), 2,4-dinitrobenzaldehyde (0.36 g, 1.2 mmol) in methanol (25 ml) was added under stirring. The resulting mixture was refluxed for 3 h and cooled to room temperature. The solid product was collected by filtration and washed with cold methanol. The microcrystalline compound was recrystallized from hot chloroform.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and with N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N).

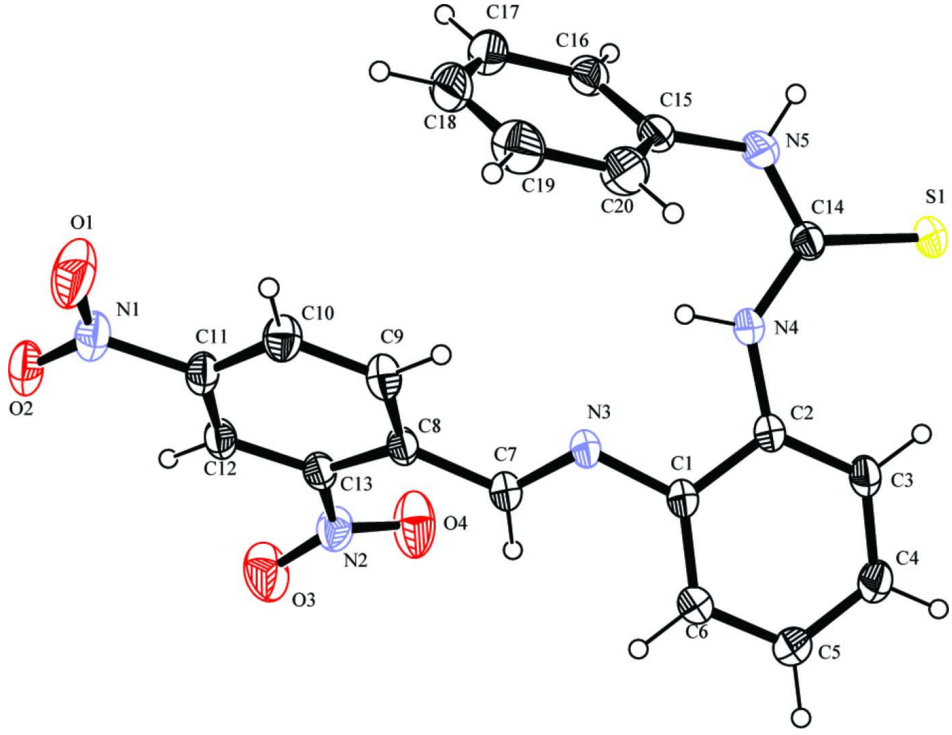

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

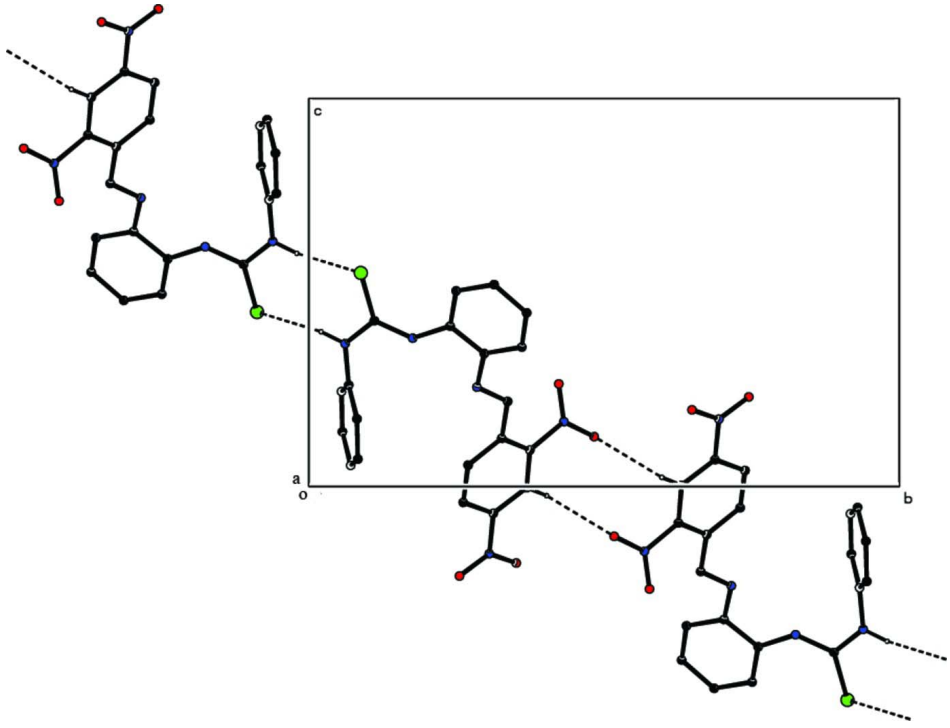

Figure 2

The packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

1-[2-(2,4-Dinitrobenzylideneamino)phenyl]-3-phenylthiourea

Crystal data

$C_{20}H_{15}N_5O_4S$
$M_r = 421.43$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.362$ (5) Å
$b = 18.767$ (3) Å
$c = 12.379$ (4) Å
$\beta = 94.827$ (5)°
$V = 1935.7$ (14) Å^3
$Z = 4$
$F(000) = 872$
$D_x = 1.446$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9702 reflections
$\theta = 2.2$–$32.3°$
$\mu = 0.21$ mm^{-1}
$T = 295$ K
Prism, orange
0.20 × 0.16 × 0.16 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.960$, $T_{max} = 0.968$
28336 measured reflections
6878 independent reflections
4509 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 32.3°$, $\theta_{min} = 2.2°$
$h = -12 \rightarrow 12$
$k = -28 \rightarrow 26$
$l = -9 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.137$
$S = 1.02$
6878 reflections
271 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
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0628P)^2 + 0.3472P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.62398 (16)	0.29698 (7)	0.34283 (10)	0.0381 (3)
C2	0.65955 (15)	0.23913 (7)	0.41328 (9)	0.0360 (3)
C3	0.76661 (18)	0.24941 (8)	0.50420 (11)	0.0448 (3)
H3	0.7860	0.2127	0.5541	0.054*
C4	0.84381 (19)	0.31360 (9)	0.52044 (12)	0.0511 (4)
H4	0.9149	0.3200	0.5816	0.061*
C5	0.8174 (2)	0.36867 (9)	0.44751 (13)	0.0560 (4)
H5	0.8740	0.4111	0.4576	0.067*
C6	0.70627 (19)	0.36049 (8)	0.35919 (12)	0.0496 (4)
H6	0.6868	0.3979	0.3106	0.060*
C7	0.42126 (16)	0.33645 (8)	0.21914 (10)	0.0412 (3)
H7	0.4321	0.3809	0.2522	0.049*
C8	0.30541 (16)	0.32650 (7)	0.12401 (10)	0.0381 (3)

C9	0.32496 (18)	0.26958 (8)	0.05491 (11)	0.0459 (3)
H9	0.4040	0.2359	0.0739	0.055*
C10	0.23061 (19)	0.26145 (9)	−0.04113 (11)	0.0478 (3)
H10	0.2441	0.2225	−0.0859	0.057*
C11	0.11616 (16)	0.31229 (8)	−0.06909 (10)	0.0425 (3)
C12	0.08777 (17)	0.36881 (8)	−0.00335 (11)	0.0424 (3)
H12	0.0087	0.4023	−0.0234	0.051*
C13	0.18123 (16)	0.37421 (8)	0.09399 (10)	0.0393 (3)
C14	0.57689 (16)	0.11081 (7)	0.42739 (10)	0.0387 (3)
C15	0.41735 (19)	0.06746 (7)	0.26115 (11)	0.0435 (3)
C16	0.2548 (2)	0.05512 (8)	0.24467 (12)	0.0471 (3)
H16	0.1955	0.0457	0.3034	0.057*
C17	0.1798 (2)	0.05672 (10)	0.14094 (14)	0.0606 (4)
H17	0.0700	0.0482	0.1298	0.073*
C18	0.2668 (3)	0.07077 (10)	0.05446 (13)	0.0687 (5)
H18	0.2161	0.0721	−0.0153	0.082*
C19	0.4278 (3)	0.08286 (11)	0.07051 (14)	0.0703 (5)
H19	0.4862	0.0923	0.0114	0.084*
C20	0.5058 (2)	0.08133 (10)	0.17423 (13)	0.0599 (4)
H20	0.6157	0.0895	0.1849	0.072*
N1	0.01932 (16)	0.30558 (9)	−0.17349 (10)	0.0534 (3)
N2	0.14010 (17)	0.43172 (8)	0.16707 (11)	0.0542 (3)
N3	0.50634 (14)	0.28461 (6)	0.25608 (9)	0.0406 (3)
N4	0.58017 (14)	0.17574 (6)	0.38222 (8)	0.0409 (3)
H4A	0.5216	0.1791	0.3219	0.049*
N5	0.49272 (17)	0.06127 (7)	0.36821 (10)	0.0529 (3)
H5A	0.4832	0.0206	0.3990	0.064*
O1	0.0455 (2)	0.25501 (10)	−0.23077 (11)	0.0917 (5)
O2	−0.08088 (15)	0.35115 (8)	−0.19739 (9)	0.0652 (3)
O3	0.0704 (2)	0.48301 (8)	0.12851 (13)	0.0930 (5)
O4	0.1705 (2)	0.42321 (9)	0.26429 (11)	0.0902 (5)
S1	0.66368 (5)	0.08789 (2)	0.55035 (3)	0.04838 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0389 (7)	0.0402 (7)	0.0341 (5)	0.0022 (5)	−0.0038 (5)	0.0060 (5)
C2	0.0366 (7)	0.0377 (7)	0.0330 (5)	0.0040 (5)	−0.0017 (5)	0.0047 (5)
C3	0.0487 (8)	0.0449 (8)	0.0384 (6)	0.0049 (6)	−0.0100 (5)	0.0062 (5)
C4	0.0529 (9)	0.0506 (9)	0.0465 (7)	0.0005 (7)	−0.0159 (6)	−0.0013 (6)
C5	0.0595 (10)	0.0439 (8)	0.0609 (9)	−0.0082 (7)	−0.0171 (7)	0.0021 (7)
C6	0.0544 (9)	0.0403 (8)	0.0516 (8)	−0.0045 (6)	−0.0108 (6)	0.0107 (6)
C7	0.0429 (7)	0.0426 (7)	0.0368 (6)	0.0018 (6)	−0.0041 (5)	0.0065 (5)
C8	0.0371 (7)	0.0428 (7)	0.0335 (5)	0.0017 (5)	−0.0012 (5)	0.0091 (5)
C9	0.0442 (8)	0.0509 (8)	0.0416 (6)	0.0108 (6)	−0.0018 (5)	0.0056 (6)
C10	0.0498 (8)	0.0550 (9)	0.0381 (6)	0.0062 (7)	0.0015 (6)	−0.0022 (6)
C11	0.0374 (7)	0.0572 (9)	0.0322 (5)	−0.0021 (6)	−0.0015 (5)	0.0077 (5)
C12	0.0375 (7)	0.0482 (8)	0.0405 (6)	0.0042 (6)	−0.0030 (5)	0.0106 (5)

C13	0.0403 (7)	0.0408 (7)	0.0364 (6)	0.0024 (6)	0.0002 (5)	0.0062 (5)
C14	0.0401 (7)	0.0392 (7)	0.0364 (6)	0.0017 (5)	−0.0001 (5)	0.0072 (5)
C15	0.0586 (9)	0.0340 (7)	0.0369 (6)	−0.0010 (6)	−0.0032 (6)	0.0032 (5)
C16	0.0558 (9)	0.0397 (7)	0.0455 (7)	0.0040 (7)	0.0019 (6)	−0.0005 (6)
C17	0.0665 (11)	0.0515 (10)	0.0602 (9)	0.0048 (8)	−0.0163 (8)	−0.0025 (7)
C18	0.1052 (16)	0.0567 (11)	0.0405 (7)	0.0006 (10)	−0.0150 (8)	−0.0024 (7)
C19	0.1034 (17)	0.0702 (12)	0.0388 (7)	−0.0056 (11)	0.0143 (9)	0.0021 (7)
C20	0.0657 (11)	0.0657 (11)	0.0489 (8)	−0.0085 (9)	0.0079 (7)	0.0050 (7)
N1	0.0498 (7)	0.0732 (10)	0.0357 (5)	−0.0006 (7)	−0.0040 (5)	0.0038 (6)
N2	0.0549 (8)	0.0525 (8)	0.0531 (7)	0.0126 (6)	−0.0072 (6)	−0.0041 (6)
N3	0.0413 (6)	0.0429 (6)	0.0360 (5)	−0.0013 (5)	−0.0064 (4)	0.0103 (4)
N4	0.0464 (6)	0.0384 (6)	0.0358 (5)	−0.0013 (5)	−0.0096 (4)	0.0074 (4)
N5	0.0704 (9)	0.0438 (7)	0.0420 (6)	−0.0131 (6)	−0.0106 (6)	0.0141 (5)
O1	0.1080 (12)	0.1083 (13)	0.0534 (7)	0.0283 (10)	−0.0248 (7)	−0.0255 (8)
O2	0.0583 (7)	0.0850 (9)	0.0490 (6)	0.0074 (6)	−0.0157 (5)	0.0116 (6)
O3	0.1231 (13)	0.0625 (9)	0.0886 (10)	0.0423 (9)	−0.0200 (9)	−0.0069 (7)
O4	0.1129 (13)	0.1065 (12)	0.0489 (7)	0.0467 (10)	−0.0073 (7)	−0.0162 (7)
S1	0.0547 (2)	0.0481 (2)	0.04016 (17)	−0.00134 (16)	−0.00860 (14)	0.01530 (14)

Geometric parameters (Å, º)

C1—C6	1.383 (2)	C12—H12	0.9300
C1—C2	1.4085 (17)	C13—N2	1.468 (2)
C1—N3	1.4132 (16)	C14—N4	1.3419 (17)
C2—C3	1.3914 (18)	C14—N5	1.3452 (19)
C2—N4	1.4003 (17)	C14—S1	1.6860 (13)
C3—C4	1.374 (2)	C15—C16	1.377 (2)
C3—H3	0.9300	C15—C20	1.381 (2)
C4—C5	1.378 (2)	C15—N5	1.4236 (17)
C4—H4	0.9300	C16—C17	1.381 (2)
C5—C6	1.383 (2)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.370 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—N3	1.2678 (17)	C18—C19	1.363 (3)
C7—C8	1.4725 (18)	C18—H18	0.9300
C7—H7	0.9300	C19—C20	1.391 (2)
C8—C9	1.387 (2)	C19—H19	0.9300
C8—C13	1.3975 (19)	C20—H20	0.9300
C9—C10	1.379 (2)	N1—O1	1.215 (2)
C9—H9	0.9300	N1—O2	1.2162 (19)
C10—C11	1.375 (2)	N2—O3	1.2031 (18)
C10—H10	0.9300	N2—O4	1.2194 (18)
C11—C12	1.370 (2)	N4—H4A	0.8600
C11—N1	1.4716 (17)	N5—H5A	0.8600
C12—C13	1.3837 (18)		
C6—C1—C2	119.82 (12)	C12—C13—N2	116.50 (12)
C6—C1—N3	123.98 (12)	C8—C13—N2	120.97 (12)

C2—C1—N3	116.18 (12)	N4—C14—N5	115.39 (11)
C3—C2—N4	126.71 (12)	N4—C14—S1	125.83 (11)
C3—C2—C1	118.81 (13)	N5—C14—S1	118.76 (10)
N4—C2—C1	114.48 (11)	C16—C15—C20	120.20 (14)
C4—C3—C2	120.16 (13)	C16—C15—N5	118.58 (13)
C4—C3—H3	119.9	C20—C15—N5	121.10 (15)
C2—C3—H3	119.9	C15—C16—C17	119.97 (15)
C3—C4—C5	120.97 (13)	C15—C16—H16	120.0
C3—C4—H4	119.5	C17—C16—H16	120.0
C5—C4—H4	119.5	C18—C17—C16	120.07 (18)
C4—C5—C6	119.67 (15)	C18—C17—H17	120.0
C4—C5—H5	120.2	C16—C17—H17	120.0
C6—C5—H5	120.2	C19—C18—C17	120.09 (15)
C5—C6—C1	120.30 (13)	C19—C18—H18	120.0
C5—C6—H6	119.9	C17—C18—H18	120.0
C1—C6—H6	119.9	C18—C19—C20	120.80 (17)
N3—C7—C8	120.17 (13)	C18—C19—H19	119.6
N3—C7—H7	119.9	C20—C19—H19	119.6
C8—C7—H7	119.9	C15—C20—C19	118.87 (18)
C9—C8—C13	116.94 (12)	C15—C20—H20	120.6
C9—C8—C7	119.16 (12)	C19—C20—H20	120.6
C13—C8—C7	123.75 (13)	O1—N1—O2	124.14 (13)
C10—C9—C8	121.91 (13)	O1—N1—C11	117.79 (14)
C10—C9—H9	119.0	O2—N1—C11	118.06 (14)
C8—C9—H9	119.0	O3—N2—O4	123.37 (15)
C11—C10—C9	118.42 (14)	O3—N2—C13	118.34 (13)
C11—C10—H10	120.8	O4—N2—C13	118.15 (13)
C9—C10—H10	120.8	C7—N3—C1	118.79 (12)
C12—C11—C10	122.65 (12)	C14—N4—C2	133.07 (11)
C12—C11—N1	118.55 (13)	C14—N4—H4A	113.5
C10—C11—N1	118.80 (14)	C2—N4—H4A	113.5
C11—C12—C13	117.43 (13)	C14—N5—C15	128.38 (12)
C11—C12—H12	121.3	C14—N5—H5A	115.8
C13—C12—H12	121.3	C15—N5—H5A	115.8
C12—C13—C8	122.50 (13)		

C6—C1—C2—C3	6.0 (2)	N5—C15—C16—C17	−176.32 (14)
N3—C1—C2—C3	−175.84 (12)	C15—C16—C17—C18	−0.2 (2)
C6—C1—C2—N4	−173.89 (14)	C16—C17—C18—C19	0.3 (3)
N3—C1—C2—N4	4.25 (18)	C17—C18—C19—C20	−0.2 (3)
N4—C2—C3—C4	175.60 (15)	C16—C15—C20—C19	0.3 (3)
C1—C2—C3—C4	−4.3 (2)	N5—C15—C20—C19	176.38 (16)
C2—C3—C4—C5	−0.2 (3)	C18—C19—C20—C15	−0.1 (3)
C3—C4—C5—C6	3.0 (3)	C12—C11—N1—O1	−179.74 (16)
C4—C5—C6—C1	−1.2 (3)	C10—C11—N1—O1	−0.1 (2)
C2—C1—C6—C5	−3.3 (2)	C12—C11—N1—O2	0.8 (2)
N3—C1—C6—C5	178.69 (15)	C10—C11—N1—O2	−179.62 (15)
N3—C7—C8—C9	−20.9 (2)	C12—C13—N2—O3	−24.3 (2)

N3—C7—C8—C13	163.79 (13)	C8—C13—N2—O3	157.70 (17)
C13—C8—C9—C10	2.3 (2)	C12—C13—N2—O4	151.72 (17)
C7—C8—C9—C10	−173.30 (14)	C8—C13—N2—O4	−26.3 (2)
C8—C9—C10—C11	1.1 (2)	C8—C7—N3—C1	175.78 (12)
C9—C10—C11—C12	−2.8 (2)	C6—C1—N3—C7	−31.3 (2)
C9—C10—C11—N1	177.57 (13)	C2—C1—N3—C7	150.61 (13)
C10—C11—C12—C13	0.9 (2)	N5—C14—N4—C2	−175.70 (14)
N1—C11—C12—C13	−179.52 (12)	S1—C14—N4—C2	5.9 (2)
C11—C12—C13—C8	2.9 (2)	C3—C2—N4—C14	2.5 (2)
C11—C12—C13—N2	−175.14 (13)	C1—C2—N4—C14	−177.57 (14)
C9—C8—C13—C12	−4.4 (2)	N4—C14—N5—C15	5.2 (2)
C7—C8—C13—C12	171.00 (13)	S1—C14—N5—C15	−176.34 (13)
C9—C8—C13—N2	173.51 (13)	C16—C15—N5—C14	−121.98 (17)
C7—C8—C13—N2	−11.1 (2)	C20—C15—N5—C14	61.8 (2)
C20—C15—C16—C17	−0.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···N3	0.86	2.14	2.614 (2)	114
C3—H3···S1	0.93	2.55	3.215 (2)	128
C7—H7···O4	0.93	2.34	2.749 (3)	106
N4—H4*A*···N3	0.86	2.14	2.614 (2)	114
N5—H5*A*···S1^{i}	0.86	2.49	3.284 (2)	155
C12—H12···O3^{ii}	0.93	2.57	3.397 (3)	148

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