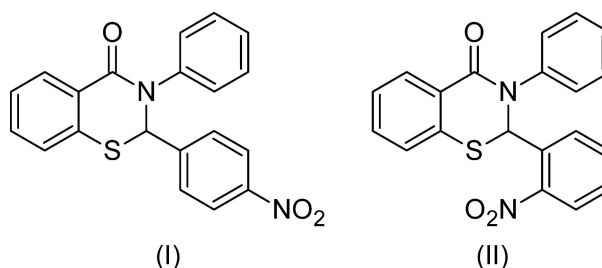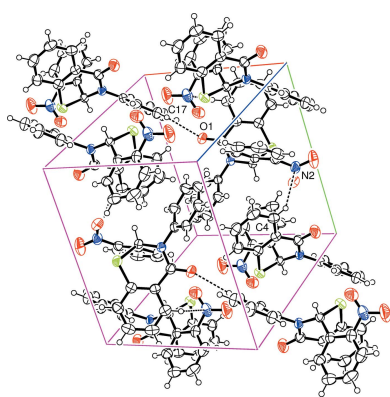# research communications

CrossMark

Crystal structures of 2-(4-nitrophenyl)-3-phenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one and 2-(2-nitrophenyl)-3-phenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one

Hemant Yennawar,[a] Aaron S. Cali,[b] Yiwen Xie[b] and Lee J. Silverberg[b]*

[a]Department of Chemistry, Pennsylvania State University, University Park, PA 16802, USA, and [b]Pennsylvania State University, Schuylkill Campus, 200 University Drive, Schuylkill Haven, PA 17972, USA. *Correspondence e-mail: ljs43@psu.edu

OPEN ACCESS

The crystal structures are reported of the isomeric compounds 2-(4-nitrophenyl)-3-phenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one, (I), and 2-(2-nitrophenyl)-3-phenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one, (II), both $C_{20}H_{14}N_2O_3S$, being the *para*-nitro and *ortho*-nitro forms, respectively, the *meta*-form of which is known [Yennawar *et al.* (2013). *Acta Cryst.* E**69**, o1679]. The six-membered thiazone ring fused with a benzene ring displays a screw-boat conformation with a total puckering amplitude of 0.627 (1) Å in (I), and a near screw-boat conformation with a total puckering amplitude of 0.600 (1) Å in (II). The dihedral angles between the planes of the substituent nitrophenyl and phenyl and rings with the benzene ring of the parent benzothiazone moiety are 75.93 (5) and 82.61 (5)° [in (I)], and 76.79 (6) and 71.66 (6)° [in (II)]. Weak intermolecular C—H···O hydrogen-bonding interactions between aromatic H-atom donors and both a nitro-O atom and a thiazone O-atom acceptor in (I) and a thiazone O atom in (II) are present, forming in (I) a centrosymmetric 22-membered cyclic dimer which is extended through a similar inversion-related 14-membered cyclic hydrogen-bonding association into a zigzag chain structure extending along *c*. In (II), a single intermolecular C—H···O hydrogen bond gives a chain structure extending along *b*. In addition, weak C—H···π interactions are present in both structures [minimum C···ring-centroid separations = 3.630 (2) and 3.581 (2) Å, respectively].

1. Chemical context

In earlier reports, we described the T3P-promoted synthesis and crystal structures of 2-(3-nitrophenyl)-3-phenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one (III) (Yennawar *et al.*, 2013) and 2,3-diphenyl-2,3-dihydro-4H-1,3-benzothiazin-4-one (IV) (Yennawar *et al.*, 2014). In compound (III), the phenyl ring substituent on the 2-position of the thiazinone ring has a nitro group in the *meta* position.

Here we report the synthesis and crystal structures of the *para*- and *ortho*-nitro analogs of $C_{20}H_{14}N_2O_3S$, the title
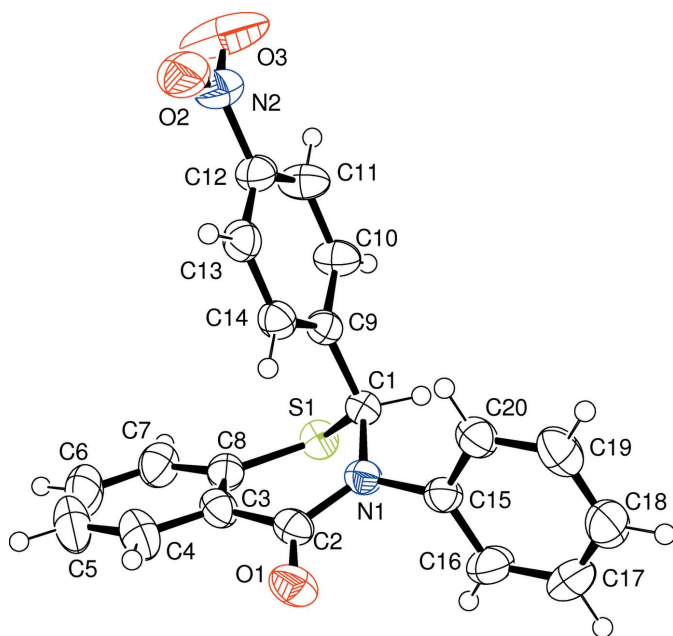
Figure 1
Molecular conformation and atom-numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level

compounds, 2-(4-nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one, (I) and (II), respectively, completing the set and allowing for comparison of the structural effects of the differently positioned nitro substituent groups.

2. Structural commentary

The crystal structures of the two racemic isomers (I) and (II) show some differences and some similarities among them-
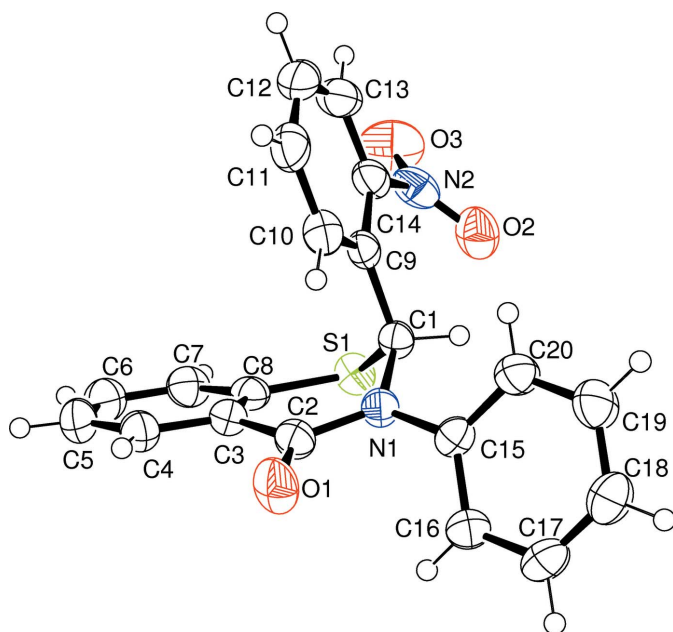
Table 1
Hydrogen-bond geometry (Å, °) for (I).

*Cg*1 and *Cg*2 are the centroids of the phenyl rings C15–C20 and C3–C8, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C20—H20···O3[i]	0.93	2.68	3.468 (2)	143
C14—H14···O1[ii]	0.93	2.65	3.4886 (17)	150
C11—H11···*Cg*1[iii]	0.93	2.85	3.646 (2)	144
C17—H17···*Cg*2[iv]	0.93	2.77	3.630 (2)	154

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

Table 2
Hydrogen-bond geometry (Å, °) for (II).

*Cg*3 is the centroid of the C15–C20 ring.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C17—H17···O1[v]	0.93	2.58	3.234 (2)	128
C6—H6···*Cg*3[vi]	0.93	2.68	3.581 (2)	163

Symmetry codes: (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

selves as well as with the *meta*-form (III) reported earlier (Yennawar *et al.*, 2013). The *para*-nitro form (I) (Fig. 1) is triclinic, space group *P*1̄, while the *ortho*-nitro form (II) (Fig. 2) is monoclinic, space group *P*2₁/*n*, as was the *meta*-form. The structures show screw-boat (I) or near screw-boat (II) conformations for the thiazine ring, as compared to an envelope conformation in the *meta*-form (III) and the unsubstituted 2,3-diphenyl compound (IV). In both (I) and (II), the three phenyl-ring planes are close to orthogonal with each other, with dihedral angles between the planes of the two substituent groups (C9–C14 = 4-nitrophenyl ring and C15–C20 = phenyl ring) with the benzene ring (C3–C8) of the parent benzothiazine moiety of 75.93 (5) and 82.61 (5)° in (I), and
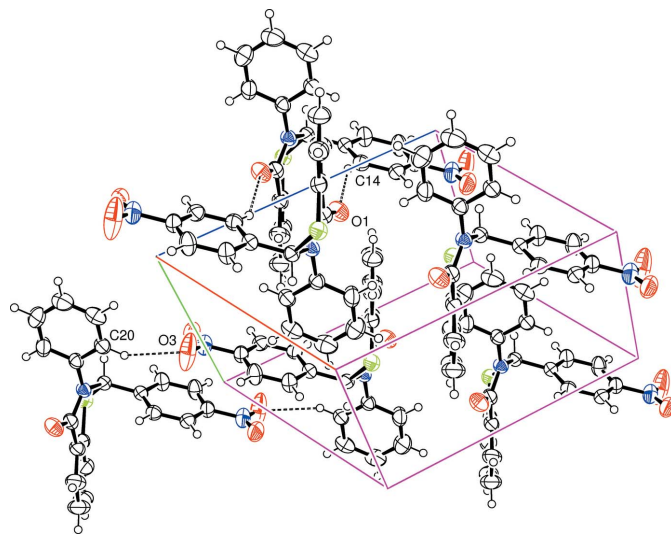

Figure 2
Molecular conformation and atom-numbering scheme for (II). Displacement ellipsoids are drawn at the 50% probability level.

Figure 3
Crystal packing in (I) showing intermolecular hydrogen-bonding interactions as dashed lines.
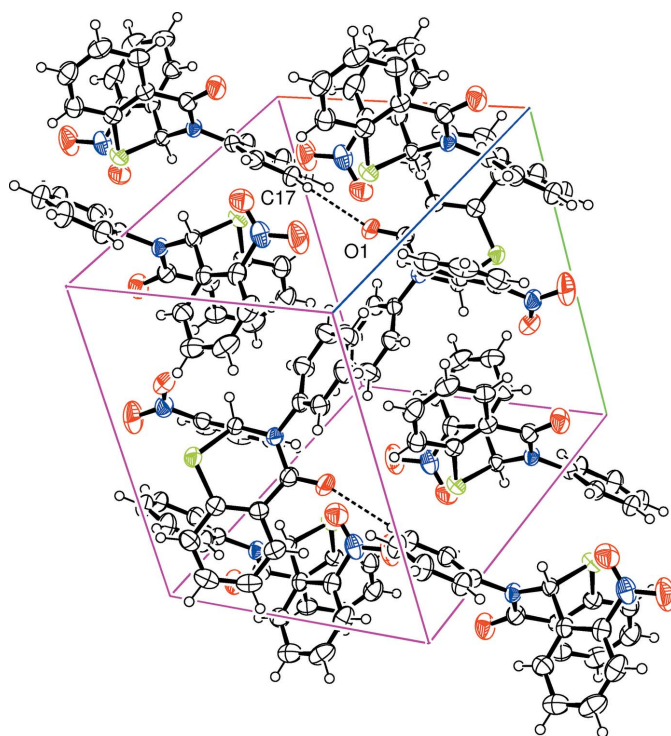
Figure 4
Crystal packing in (II) showing intermolecular hydrogen-bonding interactions as dashed lines.

76.79 (6) and 71.66 (6)° in (II), compared with 81.33 (15) and 75.73 (15)° in the *meta*-isomer (III) and 76.96 (5) and

88.99 (6)° in the unsubstituted 2,3-diphenyl compound (IV) (Yennawar *et al.*, 2014).

3. Supramolecular features

In (I), as in the *meta*-form (Yennawar *et al.*, 2013), one of the O atoms of the nitro group accepts a weak aromatic C20—H20···O3^i hydrogen bond (Table 1), forming a large centrosymmetric cyclic dimer through an $R_2^2(22)$ association. A further set of weak inversion-related C14—H14···O1^{ii} interactions with carbonyl O-atom acceptors give a second cyclic dimer [graph set $R_2^2(14)$], forming a zigzag chain structure extending along *c* (Fig. 3). In (II), a weak intermolecular C17—H17···O1^{iii} hydrogen bond to the thiazinone O-atom acceptor (Table 2) gives rise to a chain extending along the *b*-axis direction (Fig. 4). In addition, C—H···π interactions are present in both (I) (Table 1) and (II) (Table 2) [minimum C···ring-centroid separations of 3.630 (2) and 3.581 (2) Å, respectively], linking the chains to form sheets in the *bc* plane in (I) and a three-dimensional structure in (II). There are no other significant interactions present in either structure.

4. Database survey

Along with 2-(3-nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one (Yennawar *et al.*, 2013), we have also previously reported the structure of the non-nitro-substituted analog 2,3-diphenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one (Yennawar *et al.*, 2014).

Table 3
Experimental details.

	(I)	(II)
Crystal data		
Chemical formula	$C_{20}H_{14}N_2O_3S$	$C_{20}H_{14}N_2O_3S$
M_r	362.39	362.39
Crystal system, space group	Triclinic, $P\bar{1}$	Monoclinic, $P2_1/n$
Temperature (K)	298	298
a, b, c (Å)	8.1787 (12), 9.6190 (14), 12.0881 (18)	10.7396 (19), 11.778 (2), 13.532 (2)
α, β, γ (°)	73.673 (3), 71.158 (3), 86.167 (3)	90, 96.933 (3), 90
V (Å^3)	863.4 (2)	1699.2 (5)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.21	0.21
Crystal size (mm)	0.22 × 0.20 × 0.11	0.24 × 0.13 × 0.13
Data collection		
Diffractometer	Bruker SMART CCD area detector	Bruker CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2001)	Multi-scan (*SADABS*; Bruker, 2001)
T_{min}, T_{max}	0.944, 0.980	0.951, 0.973
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6717, 4134, 3740	15447, 4192, 3307
R_{int}	0.011	0.027
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.667	0.667
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.114, 1.04	0.051, 0.128, 1.03
No. of reflections	4134	4192
No. of parameters	235	235
H-atom treatment	H-atom parameters constrained	H-atom parameters not refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.27, −0.22	0.32, −0.24

Computer programs: *SMART* and *SAINT* (Bruker, 2001), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

5. Synthesis and crystallization

The syntheses were achieved in the manner previously reported, by condensation of thiosalicylic acid with a diaryl imine (Yennawar *et al.*, 2013, 2014), as follows:

A two-necked 25 ml round-bottomed flask was oven-dried, cooled under N_2, and charged with a stir bar and the imine (6 mmol). Tetrahydrofuran (2.3 ml) was added, the solid dissolved, and the solution was stirred. Pyridine (1.95 ml, 24 mmol) was added after which thiosalicylic acid (0.93 g, 6 mmol) was added. Finally, 2,4,6-tripropyl-1,3,5,2,4,6-trioxa-triphosphorinane 2,4,6-trioxide (T3P) in 2-methyltetrahydro-furan (50% *w*/*w*; 7.3 ml, 12 mmol) was added. The reaction was stirred at room temperature and followed by TLC. The mixture was poured into a separatory funnel with dichloro-methane and distilled water. The layers were separated and the aqueous fraction was then extracted twice with dichloro-methane. The organic fractions were combined and washed with saturated aqueous solutions of sodium bicarbonate and then saturated sodium chloride. The organic fraction was dried over sodium sulfate and concentrated under vacuum. The crude solid was chromatographed on 30 g flash silica gel and then recrystallized as described below.

(I): 2-(4-Nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzo-thiazin-4-one: Recrystallized twice, first from ethanol and then from hexanes. Yield: 0.162 g (7.4%); m.p. 453–456 K. $R_f = 0.55$ (40% ethyl acetate/hexanes). Crystals for X-ray crystal-lography were grown by slow evaporation from ethanol.

(II): 2-(2-Nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzo-thiazin-4-one: Recrystallized from ethanol. Yield: 0.301 g (13.8%); m.p. 445–450 K. $R_f = 0.33$ (30% ethyl acetate/hexanes). Crystals for X-ray crystallography were grown by slow evaporation from ethyl acetate.

6. Refinement details

Crystal data, data collection and structure refinement details for structures (I) and (II) are summarized in Table 3. The H atoms were placed geometrically, with C—H = 0.93–0.97 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yennawar, H. P., Bendinsky, R. V., Coyle, D. J., Cali, A. S. & Silverberg, L. J. (2014). *Acta Cryst.* E**70**, o465.
Yennawar, H. P., Silverberg, L. J., Minehan, M. J. & Tierney, J. (2013). *Acta Cryst.* E**69**, o1679.

Crystal structures of 2-(4-nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothia-zin-4-one and 2-(2-nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one

Hemant Yennawar, Aaron S. Cali, Yiwen Xie and Lee J. Silverberg

Computing details

For both compounds, data collection: *SMART* (Bruker, 2001). Cell refinement: *SAINT* (Bruker, 2001) for (I); *SMART* (Bruker, 2001) for (II). For both compounds, data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009). Software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009) for (I); *SHELXTL* (Sheldrick, 2008) for (II).

(I) 2-(4-Nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one

Crystal data

$C_{20}H_{14}N_2O_3S$	$Z = 2$
$M_r = 362.39$	$F(000) = 376$
Triclinic, $P\overline{1}$	$D_x = 1.394$ Mg m^{-3}
Hall symbol: -P 1	Melting point = 453–456 K
$a = 8.1787$ (12) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 9.6190$ (14) Å	Cell parameters from 4358 reflections
$c = 12.0881$ (18) Å	$\theta = 2.5$–28.3°
$\alpha = 73.673$ (3)°	$\mu = 0.21$ mm^{-1}
$\beta = 71.158$ (3)°	$T = 298$ K
$\gamma = 86.167$ (3)°	Block, colorless
$V = 863.4$ (2) Å^3	$0.22 \times 0.20 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	6717 measured reflections
Radiation source: fine-focus sealed tube	4134 independent reflections
Graphite monochromator	3740 reflections with $I > 2\sigma(I)$
Detector resolution: 8.34 pixels mm^{-1}	$R_{int} = 0.011$
φ and ω scans	$\theta_{max} = 28.3°$, $\theta_{min} = 1.9°$
Absorption correction: multi-scan (SADABS;Bruker, 2001)	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -15 \rightarrow 16$
$T_{min} = 0.944$, $T_{max} = 0.980$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.114$	
$S = 1.04$	H-atom parameters constrained
4134 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.1897P]$ where $P = (F_o^2 + 2F_c^2)/3$
235 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.27$ e Å^{-3}
	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.40466 (16)	0.89852 (13)	0.24333 (11)	0.0341 (2)
H1	0.4994	0.9538	0.1750	0.041*
C2	0.24767 (17)	0.93163 (15)	0.44754 (11)	0.0391 (3)
C3	0.20773 (17)	0.77262 (15)	0.49057 (12)	0.0410 (3)
C4	0.0634 (2)	0.7216 (2)	0.59206 (15)	0.0564 (4)
H4	−0.0095	0.7869	0.6269	0.068*
C5	0.0280 (2)	0.5748 (2)	0.64110 (17)	0.0680 (5)
H5	−0.0695	0.5418	0.7081	0.082*
C6	0.1362 (3)	0.47728 (19)	0.59128 (18)	0.0648 (5)
H6	0.1130	0.3784	0.6262	0.078*
C7	0.2786 (2)	0.52435 (16)	0.49030 (16)	0.0524 (4)
H7	0.3506	0.4577	0.4566	0.063*
C8	0.31425 (17)	0.67210 (15)	0.43888 (12)	0.0401 (3)
C9	0.26990 (16)	0.87025 (13)	0.18964 (11)	0.0341 (2)
C10	0.32579 (18)	0.81159 (17)	0.09111 (13)	0.0453 (3)
H10	0.4421	0.7916	0.0610	0.054*
C11	0.2116 (2)	0.78271 (18)	0.03749 (14)	0.0506 (4)
H11	0.2490	0.7427	−0.0279	0.061*
C12	0.03947 (18)	0.81485 (15)	0.08353 (13)	0.0426 (3)
C13	−0.01978 (17)	0.87506 (15)	0.17920 (12)	0.0417 (3)
H13	−0.1357	0.8970	0.2075	0.050*
C14	0.09643 (17)	0.90258 (14)	0.23300 (12)	0.0382 (3)
H14	0.0583	0.9428	0.2982	0.046*
C15	0.40376 (17)	1.13574 (13)	0.28246 (11)	0.0365 (3)
C16	0.5298 (2)	1.18389 (18)	0.31737 (16)	0.0568 (4)

H16	0.5749	1.1211	0.3736	0.068*
C17	0.5879 (3)	1.3269 (2)	0.26738 (18)	0.0690 (5)
H17	0.6711	1.3606	0.2915	0.083*
C18	0.5242 (3)	1.41946 (17)	0.18278 (15)	0.0614 (4)
H18	0.5650	1.5150	0.1492	0.074*
C19	0.4004 (2)	1.37082 (17)	0.14789 (14)	0.0547 (4)
H19	0.3571	1.4336	0.0906	0.066*
C20	0.33929 (19)	1.22879 (16)	0.19738 (12)	0.0440 (3)
H20	0.2551	1.1961	0.1735	0.053*
N1	0.34692 (14)	0.98628 (11)	0.32873 (9)	0.0368 (2)
N2	−0.08292 (19)	0.78339 (17)	0.02700 (13)	0.0568 (3)
O1	0.19567 (15)	1.00925 (12)	0.51528 (9)	0.0529 (3)
O2	−0.22860 (15)	0.82895 (17)	0.05535 (12)	0.0707 (4)
O3	−0.0330 (2)	0.7167 (3)	−0.0480 (2)	0.1181 (8)
S1	0.49691 (4)	0.73128 (4)	0.31028 (3)	0.04094 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0348 (6)	0.0353 (6)	0.0318 (6)	0.0012 (5)	−0.0101 (5)	−0.0094 (5)
C2	0.0393 (6)	0.0450 (7)	0.0332 (6)	0.0048 (5)	−0.0138 (5)	−0.0093 (5)
C3	0.0388 (6)	0.0456 (7)	0.0347 (6)	0.0016 (5)	−0.0123 (5)	−0.0041 (5)
C4	0.0453 (8)	0.0621 (9)	0.0467 (8)	0.0013 (7)	−0.0056 (6)	−0.0021 (7)
C5	0.0507 (9)	0.0703 (11)	0.0587 (10)	−0.0111 (8)	−0.0054 (8)	0.0090 (9)
C6	0.0646 (10)	0.0487 (9)	0.0688 (11)	−0.0133 (8)	−0.0243 (9)	0.0098 (8)
C7	0.0548 (9)	0.0413 (7)	0.0595 (9)	−0.0001 (6)	−0.0244 (7)	−0.0035 (6)
C8	0.0381 (6)	0.0409 (7)	0.0405 (7)	0.0000 (5)	−0.0170 (5)	−0.0046 (5)
C9	0.0367 (6)	0.0336 (6)	0.0319 (6)	0.0023 (5)	−0.0120 (5)	−0.0079 (5)
C10	0.0407 (7)	0.0593 (8)	0.0430 (7)	0.0136 (6)	−0.0167 (6)	−0.0241 (6)
C11	0.0530 (8)	0.0646 (9)	0.0479 (8)	0.0154 (7)	−0.0239 (7)	−0.0306 (7)
C12	0.0445 (7)	0.0454 (7)	0.0425 (7)	0.0000 (6)	−0.0212 (6)	−0.0102 (6)
C13	0.0340 (6)	0.0467 (7)	0.0407 (7)	−0.0005 (5)	−0.0102 (5)	−0.0079 (6)
C14	0.0374 (6)	0.0417 (6)	0.0340 (6)	0.0014 (5)	−0.0080 (5)	−0.0118 (5)
C15	0.0420 (6)	0.0358 (6)	0.0334 (6)	0.0015 (5)	−0.0128 (5)	−0.0115 (5)
C16	0.0738 (11)	0.0524 (8)	0.0566 (9)	−0.0065 (8)	−0.0390 (8)	−0.0114 (7)
C17	0.0899 (13)	0.0618 (10)	0.0694 (11)	−0.0207 (9)	−0.0350 (10)	−0.0233 (9)
C18	0.0889 (13)	0.0397 (7)	0.0505 (9)	−0.0095 (8)	−0.0105 (8)	−0.0156 (7)
C19	0.0682 (10)	0.0441 (8)	0.0421 (8)	0.0071 (7)	−0.0120 (7)	−0.0044 (6)
C20	0.0447 (7)	0.0478 (7)	0.0372 (7)	0.0013 (6)	−0.0141 (6)	−0.0070 (6)
N1	0.0433 (6)	0.0359 (5)	0.0319 (5)	−0.0005 (4)	−0.0117 (4)	−0.0104 (4)
N2	0.0553 (8)	0.0679 (9)	0.0579 (8)	0.0003 (6)	−0.0305 (7)	−0.0190 (7)
O1	0.0624 (7)	0.0565 (6)	0.0385 (5)	0.0077 (5)	−0.0104 (5)	−0.0191 (5)
O2	0.0425 (6)	0.1119 (11)	0.0615 (7)	−0.0054 (6)	−0.0213 (5)	−0.0225 (7)
O3	0.1007 (13)	0.1719 (19)	0.1604 (18)	0.0508 (12)	−0.0875 (13)	−0.1248 (17)
S1	0.03605 (18)	0.04201 (19)	0.04357 (19)	0.00672 (13)	−0.01346 (14)	−0.01027 (14)

Geometric parameters (Å, º)

C1—N1	1.4570 (15)	C11—C12	1.386 (2)
C1—C9	1.5203 (17)	C11—H11	0.9300
C1—S1	1.8200 (13)	C12—C13	1.373 (2)
C1—H1	0.9800	C12—N2	1.4695 (18)
C2—O1	1.2186 (17)	C13—C14	1.3878 (19)
C2—N1	1.3702 (17)	C13—H13	0.9300
C2—C3	1.4921 (19)	C14—H14	0.9300
C3—C4	1.394 (2)	C15—C20	1.3807 (19)
C3—C8	1.400 (2)	C15—C16	1.3817 (19)
C4—C5	1.379 (3)	C15—N1	1.4371 (16)
C4—H4	0.9300	C16—C17	1.385 (2)
C5—C6	1.374 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.371 (3)
C6—C7	1.376 (3)	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.368 (3)
C7—C8	1.390 (2)	C18—H18	0.9300
C7—H7	0.9300	C19—C20	1.383 (2)
C8—S1	1.7574 (14)	C19—H19	0.9300
C9—C14	1.3916 (18)	C20—H20	0.9300
C9—C10	1.3920 (18)	N2—O3	1.205 (2)
C10—C11	1.377 (2)	N2—O2	1.2166 (19)
C10—H10	0.9300		
N1—C1—C9	114.94 (10)	C12—C11—H11	120.9
N1—C1—S1	110.58 (8)	C13—C12—C11	122.37 (12)
C9—C1—S1	111.83 (8)	C13—C12—N2	119.26 (13)
N1—C1—H1	106.3	C11—C12—N2	118.37 (13)
C9—C1—H1	106.3	C12—C13—C14	118.81 (13)
S1—C1—H1	106.3	C12—C13—H13	120.6
O1—C2—N1	121.47 (13)	C14—C13—H13	120.6
O1—C2—C3	121.52 (12)	C13—C14—C9	120.22 (12)
N1—C2—C3	117.00 (11)	C13—C14—H14	119.9
C4—C3—C8	118.67 (14)	C9—C14—H14	119.9
C4—C3—C2	118.08 (13)	C20—C15—C16	120.19 (13)
C8—C3—C2	123.11 (12)	C20—C15—N1	119.55 (12)
C5—C4—C3	120.44 (17)	C16—C15—N1	120.15 (12)
C5—C4—H4	119.8	C15—C16—C17	119.06 (15)
C3—C4—H4	119.8	C15—C16—H16	120.5
C6—C5—C4	120.23 (16)	C17—C16—H16	120.5
C6—C5—H5	119.9	C18—C17—C16	120.85 (16)
C4—C5—H5	119.9	C18—C17—H17	119.6
C5—C6—C7	120.67 (16)	C16—C17—H17	119.6
C5—C6—H6	119.7	C19—C18—C17	119.80 (15)
C7—C6—H6	119.7	C19—C18—H18	120.1
C6—C7—C8	119.64 (16)	C17—C18—H18	120.1
C6—C7—H7	120.2	C18—C19—C20	120.37 (15)

C8—C7—H7	120.2	C18—C19—H19	119.8
C7—C8—C3	120.31 (14)	C20—C19—H19	119.8
C7—C8—S1	119.34 (12)	C15—C20—C19	119.72 (14)
C3—C8—S1	120.34 (10)	C15—C20—H20	120.1
C14—C9—C10	119.35 (12)	C19—C20—H20	120.1
C14—C9—C1	123.12 (11)	C2—N1—C15	120.70 (10)
C10—C9—C1	117.53 (11)	C2—N1—C1	123.15 (11)
C11—C10—C9	121.02 (13)	C15—N1—C1	116.13 (10)
C11—C10—H10	119.5	O3—N2—O2	122.84 (14)
C9—C10—H10	119.5	O3—N2—C12	118.39 (15)
C10—C11—C12	118.22 (13)	O2—N2—C12	118.73 (14)
C10—C11—H11	120.9	C8—S1—C1	96.00 (6)

O1—C2—C3—C4	22.9 (2)	C20—C15—C16—C17	1.1 (3)
N1—C2—C3—C4	−157.74 (13)	N1—C15—C16—C17	177.15 (16)
O1—C2—C3—C8	−152.79 (14)	C15—C16—C17—C18	−1.2 (3)
N1—C2—C3—C8	26.57 (18)	C16—C17—C18—C19	0.7 (3)
C8—C3—C4—C5	0.8 (2)	C17—C18—C19—C20	−0.1 (3)
C2—C3—C4—C5	−175.10 (15)	C16—C15—C20—C19	−0.5 (2)
C3—C4—C5—C6	0.9 (3)	N1—C15—C20—C19	−176.61 (13)
C4—C5—C6—C7	−1.6 (3)	C18—C19—C20—C15	0.0 (2)
C5—C6—C7—C8	0.6 (3)	O1—C2—N1—C15	4.6 (2)
C6—C7—C8—C3	1.1 (2)	C3—C2—N1—C15	−174.72 (11)
C6—C7—C8—S1	179.73 (13)	O1—C2—N1—C1	−176.96 (12)
C4—C3—C8—C7	−1.8 (2)	C3—C2—N1—C1	3.67 (18)
C2—C3—C8—C7	173.91 (13)	C20—C15—N1—C2	−112.20 (14)
C4—C3—C8—S1	179.59 (11)	C16—C15—N1—C2	71.69 (18)
C2—C3—C8—S1	−4.74 (18)	C20—C15—N1—C1	69.30 (16)
N1—C1—C9—C14	−10.83 (17)	C16—C15—N1—C1	−106.80 (15)
S1—C1—C9—C14	116.32 (12)	C9—C1—N1—C2	79.64 (15)
N1—C1—C9—C10	167.99 (12)	S1—C1—N1—C2	−48.15 (14)
S1—C1—C9—C10	−64.86 (14)	C9—C1—N1—C15	−101.90 (12)
C14—C9—C10—C11	−1.2 (2)	S1—C1—N1—C15	130.31 (10)
C1—C9—C10—C11	179.93 (13)	C13—C12—N2—O3	−172.21 (19)
C9—C10—C11—C12	0.6 (2)	C11—C12—N2—O3	8.0 (3)
C10—C11—C12—C13	0.6 (2)	C13—C12—N2—O2	9.7 (2)
C10—C11—C12—N2	−179.65 (14)	C11—C12—N2—O2	−170.08 (16)
C11—C12—C13—C14	−1.1 (2)	C7—C8—S1—C1	148.50 (12)
N2—C12—C13—C14	179.16 (12)	C3—C8—S1—C1	−32.84 (12)
C12—C13—C14—C9	0.4 (2)	N1—C1—S1—C8	56.20 (9)
C10—C9—C14—C13	0.7 (2)	C9—C1—S1—C8	−73.27 (9)
C1—C9—C14—C13	179.49 (12)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg2 are the centroids of the phenyl rings C15–C20 and C3–C8, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C20—H20···O3[i]	0.93	2.68	3.468 (2)	143

C1—H1···O2ⁱⁱ	0.98	2.65	3.2851 (18)	123
C14—H14···O1ⁱⁱⁱ	0.93	2.65	3.4886 (17)	150
C11—H11···*Cg*1ⁱᵛ	0.93	2.85	3.646 (2)	144
C17—H17···*Cg*2ᵛ	0.93	2.77	3.630 (2)	154

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

(II) 2-(2-Nitrophenyl)-3-phenyl-2,3-dihydro-4*H*-1,3-benzothiazin-4-one

Crystal data

$C_{20}H_{14}N_2O_3S$	$F(000) = 752$
$M_r = 362.39$	$D_x = 1.417$ Mg m⁻³
Monoclinic, $P2_1/n$	Melting point = 445–450 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 10.7396$ (19) Å	Cell parameters from 4222 reflections
$b = 11.778$ (2) Å	$\theta = 2.3–28.2°$
$c = 13.532$ (2) Å	$\mu = 0.21$ mm⁻¹
$\beta = 96.933$ (3)°	$T = 298$ K
$V = 1699.2$ (5) Å³	Block, colorless
$Z = 4$	0.24 × 0.13 × 0.13 mm

Data collection

Bruker CCD area-detector diffractometer	15447 measured reflections
Radiation source: fine-focus sealed tube	4192 independent reflections
Graphite monochromator	3307 reflections with $I > 2\sigma(I)$
Detector resolution: 8.34 pixels mm⁻¹	$R_{int} = 0.027$
φ and ω scans	$\theta_{max} = 28.3°, \theta_{min} = 2.3°$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = −14→14$
	$k = −15→14$
$T_{min} = 0.951, T_{max} = 0.973$	$l = −17→17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.128$	
$S = 1.03$	H-atom parameters not refined
4192 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.429P]$
235 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.32$ e Å⁻³
	$\Delta\rho_{min} = −0.24$ e Å⁻³

Special details

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.28981 (14)	0.46215 (14)	0.18506 (13)	0.0331 (4)
H1	0.2834	0.5426	0.2022	0.040*
C2	0.46574 (15)	0.33061 (16)	0.16797 (14)	0.0397 (4)
C3	0.37791 (15)	0.26178 (15)	0.09805 (13)	0.0366 (4)
C4	0.40908 (18)	0.14818 (16)	0.08454 (14)	0.0436 (4)
H4	0.4780	0.1169	0.1233	0.052*
C5	0.3393 (2)	0.08211 (18)	0.01489 (16)	0.0522 (5)
H5	0.3592	0.0059	0.0082	0.063*
C6	0.2394 (2)	0.12935 (19)	−0.04536 (16)	0.0533 (5)
H6	0.1943	0.0853	−0.0942	0.064*
C7	0.20612 (18)	0.24112 (18)	−0.03363 (14)	0.0468 (5)
H7	0.1388	0.2723	−0.0744	0.056*
C8	0.27389 (16)	0.30731 (15)	0.03961 (13)	0.0374 (4)
C9	0.21338 (14)	0.39669 (14)	0.25355 (12)	0.0335 (4)
C10	0.27005 (18)	0.31979 (15)	0.32244 (14)	0.0429 (4)
H10	0.3563	0.3091	0.3270	0.051*
C11	0.2016 (2)	0.25840 (18)	0.38472 (14)	0.0522 (5)
H11	0.2424	0.2082	0.4309	0.063*
C12	0.0733 (2)	0.2715 (2)	0.37837 (16)	0.0591 (6)
H12	0.0274	0.2296	0.4196	0.071*
C13	0.0137 (2)	0.3465 (2)	0.31115 (16)	0.0545 (5)
H13	−0.0729	0.3552	0.3060	0.065*
C14	0.08287 (16)	0.40890 (17)	0.25134 (13)	0.0402 (4)
C15	0.50767 (15)	0.51223 (15)	0.25360 (13)	0.0353 (4)
C16	0.62065 (16)	0.53924 (16)	0.21859 (14)	0.0408 (4)
H16	0.6429	0.5045	0.1615	0.049*
C17	0.69952 (17)	0.61808 (18)	0.26934 (15)	0.0474 (5)
H17	0.7754	0.6358	0.2465	0.057*
C18	0.66703 (19)	0.67052 (19)	0.35309 (16)	0.0533 (5)
H18	0.7207	0.7234	0.3868	0.064*
C19	0.55443 (19)	0.6444 (2)	0.38714 (16)	0.0545 (5)
H19	0.5319	0.6805	0.4435	0.065*
C20	0.47462 (17)	0.56458 (17)	0.33784 (15)	0.0455 (5)
H20	0.3993	0.5465	0.3615	0.055*
N1	0.42334 (12)	0.43381 (12)	0.19877 (11)	0.0357 (3)
N2	0.01309 (14)	0.49390 (17)	0.18749 (13)	0.0497 (4)
O1	0.57182 (12)	0.29780 (12)	0.19525 (12)	0.0591 (4)
O2	0.06296 (14)	0.58460 (14)	0.17327 (12)	0.0602 (4)
O3	−0.09447 (14)	0.47116 (19)	0.15352 (15)	0.0854 (6)
S1	0.22755 (4)	0.44863 (4)	0.05436 (3)	0.04088 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0288 (7)	0.0318 (9)	0.0379 (9)	0.0023 (6)	0.0007 (6)	−0.0011 (7)

C2	0.0333 (8)	0.0393 (10)	0.0466 (10)	0.0038 (7)	0.0054 (7)	−0.0010 (8)
C3	0.0377 (8)	0.0358 (9)	0.0373 (9)	−0.0005 (7)	0.0088 (7)	−0.0009 (7)
C4	0.0498 (10)	0.0381 (10)	0.0446 (10)	0.0029 (8)	0.0120 (8)	0.0015 (8)
C5	0.0664 (13)	0.0383 (11)	0.0544 (12)	−0.0044 (9)	0.0179 (10)	−0.0094 (9)
C6	0.0589 (12)	0.0542 (13)	0.0473 (11)	−0.0127 (10)	0.0090 (9)	−0.0137 (10)
C7	0.0466 (10)	0.0545 (12)	0.0391 (10)	−0.0037 (9)	0.0039 (8)	−0.0051 (9)
C8	0.0383 (8)	0.0416 (10)	0.0339 (9)	−0.0012 (7)	0.0104 (7)	0.0013 (7)
C9	0.0336 (8)	0.0312 (9)	0.0353 (8)	0.0002 (6)	0.0031 (6)	−0.0078 (7)
C10	0.0483 (10)	0.0380 (10)	0.0419 (10)	0.0031 (8)	0.0039 (8)	−0.0018 (8)
C11	0.0805 (14)	0.0378 (11)	0.0394 (10)	−0.0037 (10)	0.0124 (10)	−0.0033 (8)
C12	0.0815 (15)	0.0509 (13)	0.0504 (12)	−0.0203 (11)	0.0305 (11)	−0.0108 (10)
C13	0.0473 (10)	0.0632 (14)	0.0563 (12)	−0.0125 (10)	0.0193 (9)	−0.0170 (11)
C14	0.0364 (8)	0.0436 (10)	0.0408 (10)	−0.0010 (7)	0.0056 (7)	−0.0112 (8)
C15	0.0299 (7)	0.0355 (9)	0.0392 (9)	−0.0010 (7)	−0.0010 (6)	0.0030 (7)
C16	0.0350 (8)	0.0454 (11)	0.0422 (10)	−0.0016 (7)	0.0050 (7)	0.0013 (8)
C17	0.0337 (8)	0.0512 (12)	0.0565 (12)	−0.0090 (8)	0.0028 (8)	0.0037 (9)
C18	0.0478 (11)	0.0530 (13)	0.0565 (12)	−0.0126 (9)	−0.0045 (9)	−0.0073 (10)
C19	0.0520 (11)	0.0595 (13)	0.0516 (12)	−0.0069 (10)	0.0049 (9)	−0.0183 (10)
C20	0.0382 (9)	0.0511 (12)	0.0479 (11)	−0.0049 (8)	0.0081 (8)	−0.0060 (9)
N1	0.0272 (6)	0.0349 (8)	0.0444 (8)	0.0005 (5)	0.0015 (6)	−0.0035 (6)
N2	0.0339 (8)	0.0658 (12)	0.0491 (10)	0.0129 (8)	0.0040 (7)	−0.0089 (9)
O1	0.0378 (7)	0.0496 (9)	0.0862 (11)	0.0134 (6)	−0.0069 (7)	−0.0107 (8)
O2	0.0572 (9)	0.0487 (9)	0.0732 (11)	0.0146 (7)	0.0014 (7)	−0.0018 (8)
O3	0.0352 (8)	0.1241 (17)	0.0925 (14)	0.0023 (9)	−0.0104 (8)	0.0063 (12)
S1	0.0424 (2)	0.0428 (3)	0.0361 (2)	0.00758 (19)	−0.00063 (18)	0.00295 (19)

Geometric parameters (Å, º)

C1—N1	1.462 (2)	C11—C12	1.379 (3)
C1—C9	1.520 (2)	C11—H11	0.9300
C1—S1	1.8207 (17)	C12—C13	1.370 (3)
C1—H1	0.9800	C12—H12	0.9300
C2—O1	1.217 (2)	C13—C14	1.375 (3)
C2—N1	1.380 (2)	C13—H13	0.9300
C2—C3	1.492 (2)	C14—N2	1.468 (3)
C3—C8	1.396 (2)	C15—C20	1.380 (3)
C3—C4	1.397 (3)	C15—C16	1.392 (2)
C4—C5	1.373 (3)	C15—N1	1.436 (2)
C4—H4	0.9300	C16—C17	1.382 (3)
C5—C6	1.384 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.372 (3)
C6—C7	1.378 (3)	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.380 (3)
C7—C8	1.395 (3)	C18—H18	0.9300
C7—H7	0.9300	C19—C20	1.388 (3)
C8—S1	1.7557 (19)	C19—H19	0.9300
C9—C10	1.387 (2)	C20—H20	0.9300
C9—C14	1.406 (2)	N2—O3	1.220 (2)

| C10—C11 | 1.386 (3) | N2—O2 | 1.221 (2) |
| C10—H10 | 0.9300 | | |

N1—C1—C9	113.60 (14)	C10—C11—H11	119.9
N1—C1—S1	110.05 (11)	C13—C12—C11	119.80 (19)
C9—C1—S1	112.70 (11)	C13—C12—H12	120.1
N1—C1—H1	106.7	C11—C12—H12	120.1
C9—C1—H1	106.7	C12—C13—C14	119.52 (19)
S1—C1—H1	106.7	C12—C13—H13	120.2
O1—C2—N1	121.25 (16)	C14—C13—H13	120.2
O1—C2—C3	121.10 (16)	C13—C14—C9	122.74 (19)
N1—C2—C3	117.63 (14)	C13—C14—N2	115.91 (17)
C8—C3—C4	118.82 (17)	C9—C14—N2	121.29 (17)
C8—C3—C2	123.50 (16)	C20—C15—C16	120.06 (16)
C4—C3—C2	117.42 (16)	C20—C15—N1	120.35 (15)
C5—C4—C3	120.90 (19)	C16—C15—N1	119.52 (16)
C5—C4—H4	119.6	C17—C16—C15	119.45 (18)
C3—C4—H4	119.6	C17—C16—H16	120.3
C4—C5—C6	119.78 (19)	C15—C16—H16	120.3
C4—C5—H5	120.1	C18—C17—C16	120.73 (18)
C6—C5—H5	120.1	C18—C17—H17	119.6
C7—C6—C5	120.66 (19)	C16—C17—H17	119.6
C7—C6—H6	119.7	C17—C18—C19	119.73 (18)
C5—C6—H6	119.7	C17—C18—H18	120.1
C6—C7—C8	119.68 (19)	C19—C18—H18	120.1
C6—C7—H7	120.2	C18—C19—C20	120.38 (19)
C8—C7—H7	120.2	C18—C19—H19	119.8
C7—C8—C3	120.08 (17)	C20—C19—H19	119.8
C7—C8—S1	118.68 (14)	C15—C20—C19	119.64 (18)
C3—C8—S1	121.22 (13)	C15—C20—H20	120.2
C10—C9—C14	115.90 (17)	C19—C20—H20	120.2
C10—C9—C1	121.04 (15)	C2—N1—C15	120.81 (13)
C14—C9—C1	123.06 (15)	C2—N1—C1	121.14 (14)
C11—C10—C9	121.84 (19)	C15—N1—C1	117.81 (13)
C11—C10—H10	119.1	O3—N2—O2	123.10 (19)
C9—C10—H10	119.1	O3—N2—C14	117.7 (2)
C12—C11—C10	120.2 (2)	O2—N2—C14	119.16 (15)
C12—C11—H11	119.9	C8—S1—C1	96.74 (8)

O1—C2—C3—C8	−158.54 (18)	C1—C9—C14—N2	−5.3 (3)
N1—C2—C3—C8	20.1 (3)	C20—C15—C16—C17	0.5 (3)
O1—C2—C3—C4	15.5 (3)	N1—C15—C16—C17	177.50 (16)
N1—C2—C3—C4	−165.94 (16)	C15—C16—C17—C18	−0.6 (3)
C8—C3—C4—C5	0.2 (3)	C16—C17—C18—C19	0.0 (3)
C2—C3—C4—C5	−174.05 (17)	C17—C18—C19—C20	0.7 (3)
C3—C4—C5—C6	2.3 (3)	C16—C15—C20—C19	0.2 (3)
C4—C5—C6—C7	−2.5 (3)	N1—C15—C20—C19	−176.78 (18)
C5—C6—C7—C8	0.1 (3)	C18—C19—C20—C15	−0.8 (3)

C6—C7—C8—C3	2.5 (3)	O1—C2—N1—C15	8.0 (3)
C6—C7—C8—S1	−178.84 (15)	C3—C2—N1—C15	−170.55 (15)
C4—C3—C8—C7	−2.7 (3)	O1—C2—N1—C1	−166.08 (17)
C2—C3—C8—C7	171.27 (16)	C3—C2—N1—C1	15.3 (2)
C4—C3—C8—S1	178.72 (13)	C20—C15—N1—C2	−133.66 (19)
C2—C3—C8—S1	−7.3 (2)	C16—C15—N1—C2	49.4 (2)
N1—C1—C9—C10	1.1 (2)	C20—C15—N1—C1	40.7 (2)
S1—C1—C9—C10	127.10 (15)	C16—C15—N1—C1	−136.33 (17)
N1—C1—C9—C14	−178.54 (15)	C9—C1—N1—C2	71.6 (2)
S1—C1—C9—C14	−52.5 (2)	S1—C1—N1—C2	−55.81 (19)
C14—C9—C10—C11	0.4 (3)	C9—C1—N1—C15	−102.67 (17)
C1—C9—C10—C11	−179.25 (16)	S1—C1—N1—C15	129.90 (13)
C9—C10—C11—C12	1.0 (3)	C13—C14—N2—O3	−35.0 (3)
C10—C11—C12—C13	−0.8 (3)	C9—C14—N2—O3	147.80 (19)
C11—C12—C13—C14	−0.7 (3)	C13—C14—N2—O2	142.80 (19)
C12—C13—C14—C9	2.1 (3)	C9—C14—N2—O2	−34.4 (3)
C12—C13—C14—N2	−175.09 (18)	C7—C8—S1—C1	153.79 (14)
C10—C9—C14—C13	−1.9 (3)	C3—C8—S1—C1	−27.57 (16)
C1—C9—C14—C13	177.69 (17)	N1—C1—S1—C8	55.42 (13)
C10—C9—C14—N2	175.12 (16)	C9—C1—S1—C8	−72.50 (13)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C15–C20 ring.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C17—H17⋯O1[i]	0.93	2.58	3.234 (2)	128
C6—H6⋯*Cg*3[ii]	0.93	2.68	3.581 (2)	163

Symmetry codes: (i) −*x*+3/2, *y*+1/2, −*z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2.