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N′-[Bis(benzylsulfanyl)methylidene]benzohydrazide. Corrigendum

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In the paper by Tayamon *et al.* [*Acta Cryst.* (2012), E**68**, o1640–o1641], the chemical name in the title is incorrect.

In the paper by Tayamon *et al.* (2012), the chemical name was given incorrectly in the title. The correct title should be '*N*′-[bis(benzylsulfanyl)methylidene]pyridine-4-carbohydrazide'. The scheme and chemical data are correct as given in the original article.

References

Tayamon, S., Ravoof, T. B. S. A., Tahir, M. I. M., Crouse, K. A. & Tiekink, E. R. T. (2012). *Acta Cryst.* E**68**, o1640–o1641.

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N′-[Bis(benzylsulfanyl)methylidene]benzohydrazide

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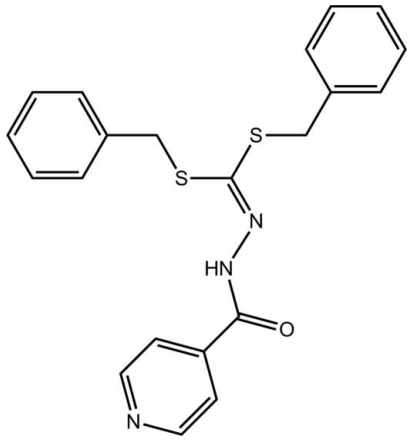
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.097; data-to-parameter ratio = 15.7.

In the title hydrazonodithioate, $C_{21}H_{19}N_3OS_2$, the amide group is twisted out of the plane through the $S_2C{=}N$ atoms: the C—N—N—C torsion angle is 139.71 (13)°. The pyridine ring forms dihedral angles of 52.96 (8) and 86.46 (8)° with the phenyl rings, and the latter are approximately orthogonal [dihedral angle = 76.42 (9)°]. Supramolecular chains sustained by N—H···O hydrogen bonds and propagated by glide symmetry along the c axis are found in the crystal structure. The chains are consolidated into a three-dimensional architecture by C—H···O and C—H···N interactions.

Related literature

For background to the coordination chemistry of dithiocarbazate derivatives, see: Tarafder *et al.* (2002); Ravoof *et al.* (2010). For related syntheses, see: Ali & Tarafder (1977); Ali *et al.* (2001); Manan *et al.* (2012). For related structures, see: Jasinski *et al.* (2010); Singh *et al.* (2007).



Experimental

Crystal data

$C_{21}H_{19}N_3OS_2$
M_r = 393.51
Monoclinic, $P2_1/c$
a = 11.2593 (4) Å
b = 21.2182 (7) Å
c = 8.6041 (3) Å
β = 103.678 (3)°
V = 1997.24 (12) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.54 mm^{-1}
T = 150 K
0.50 × 0.36 × 0.16 mm

Data collection

Agilent Xcaliber Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.42, T_{max} = 0.67
38338 measured reflections
3867 independent reflections
3715 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.097
S = 1.03
3867 reflections
247 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···O1^{i}	0.864 (17)	1.936 (17)	2.7852 (15)	167.4 (16)
C7—H7···N3^{ii}	0.95	2.54	3.339 (2)	142
C8—H8···N3^{iii}	0.95	2.52	3.424 (2)	158
C18—H18···O1^{i}	0.95	2.53	3.365 (2)	147

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Support for the project came from Universiti Putra Malaysia (UPM) under their Research University Grant Scheme (RUGS No. 9174000), the Malaysian Ministry of Science, Technology and Innovation (grant No. 09-02-04-0752-EA001) and the Malaysian Fundamental Research Grant Scheme (FRGS No. 01-13-11-986FR). We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (grant No. UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6755).

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supporting information

Acta Cryst. (2012). E**68**, o1640–o1641 [doi:10.1107/S1600536812019472]

N′-[Bis(benzylsulfanyl)methylidene]benzohydrazide

Shahedeh Tayamon, Thahira Begum S. A. Ravoof, Mohamed Ibrahim Mohamed Tahir, Karen A. Crouse and Edward R. T. Tiekink

S1. Comment

Our interest in investigating the coordination properties of ligands containing the H—N—C═S moiety (Tarafder *et al.*, 2002; Ravoof *et al.*, 2010) and our desire to expand the study of this class of biologically important compounds has lead us to synthesize a series of related ligands (Ali *et al.*, 2001; Manan *et al.*, 2012). The title compound *N*′-bis(benzylsulfanyl)methylidene]benzohydrazide, (I), was obtained from an attempt to prepare *S*-benzyl isonicotinoylcarbonohydrazonodithioate (see *Experimental*).

In (I), Fig. 1, the amide is twisted out of the plane through the S_2C═N atoms with the C1—N1—N2—C16 torsion angle being 139.71 (13)°. A similar twist was found in the structure of $(PhCH_2S)_2C$═NN(H)C(═O)C_6H_4OMe-4 (Jasinski *et al.*, 2010) but a planar arrangement was observed in the structure of $(PhCH_2S)_2C$═NN(H)C(═O)C_6H_4OMe-2 (Singh *et al.*, 2007). The dihedral angle between the phenyl rings is 76.42 (9)°, indicating an almost orthogonal relationship. Each of these rings forms a dihedral angle of 52.96 (8) and 86.46 (8)° with the pyridyl ring.

The crystal packing features supramolecular chains sustained by N—H···O hydrogen bonds, Table 1, and propagated by glide symmetry along the *c* axis, Fig. 2. Chains are consolidated into a three-dimensional architecture by C—H···O and C—H···N interactions, Fig. 3 and Table 1.

S2. Experimental

The procedure to synthesize *S*-benzyldithiocarbazate (Ali & Tarafder, 1977) was adapted to prepare *S*-benzyl isonicotinoylcarbonohydrazono dithioate by replacing hydrazine with its isonicotinic acid derivative. Potassium hydroxide (0.2 mol, 11.2 g) in absolute ethanol (70 ml) was added to a suspension of isonicotinic acid hydrazide (0.2 mol, 27.43 g) in absolute ethanol (700 ml). The pale-yellow solution was kept in an ice-salt bath and carbon disulfide (0.2 mol) was added drop-wise with constant stirring over one hour. Benzylchloride (0.2 mol, 23 ml) was then added drop-wise with vigorous stirring to the pale-orange solution obtained above. The reaction temperature was maintained below 278 K. An unidentified pale-yellow solid (33.84 g) which did not contain any benzyl substituent was filtered from the mixture. The filtrate was kept in a freezer for one week before it was used as replacement for absolute ethanol to repeat the above reaction. The final solution produced dark-yellow blocks of the title compound after storage at 268 K for 5 months. (Yield 16 g; *M*.pt: 369 K).

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H = 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{equiv}(C). The amino H-atom was refined with a distance restraint of N—H = 0.88±0.01 Å, and with U_{iso}(H) = 1.2U_{eq}(N).

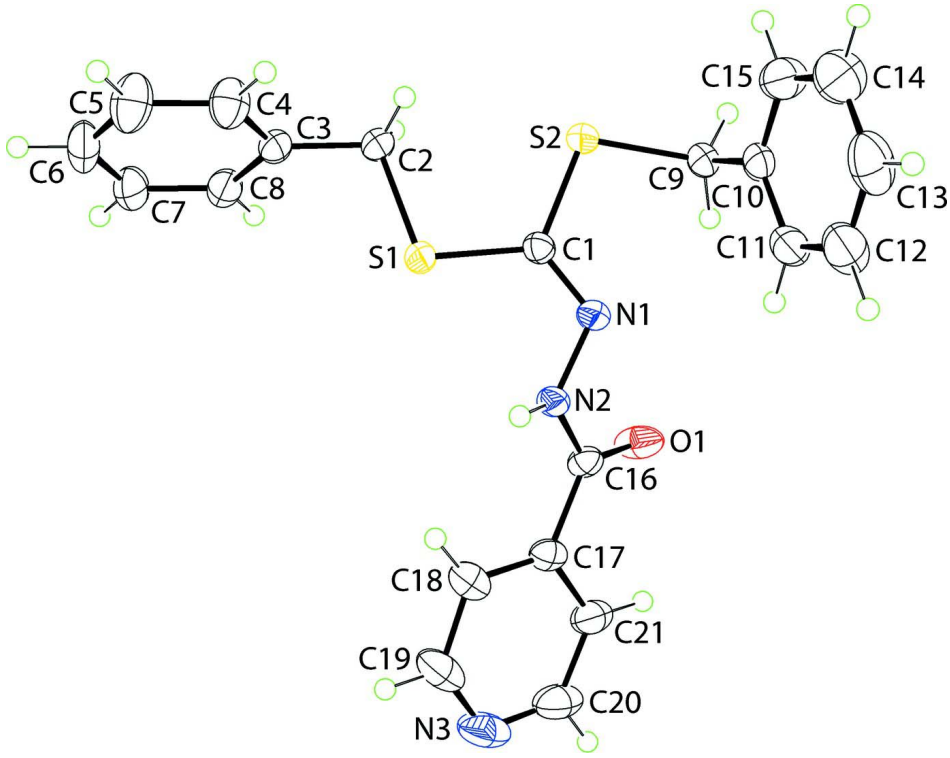

Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 50% probability level.

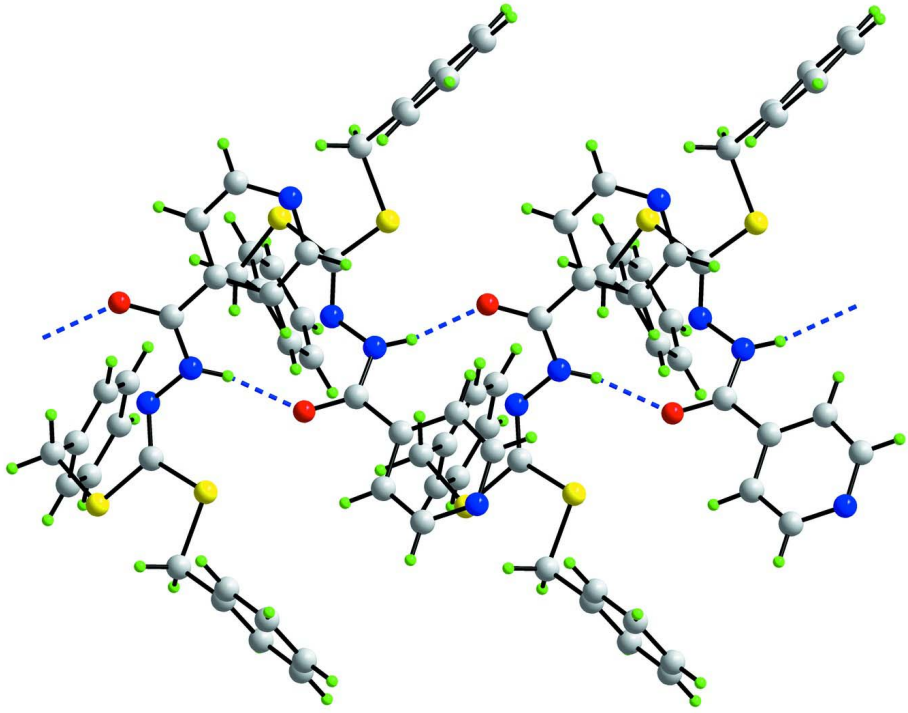

Figure 2

A view of the supramolecular chain in (I) mediated by N—H···O hydrogen bonding, shown as blue dashed lines.

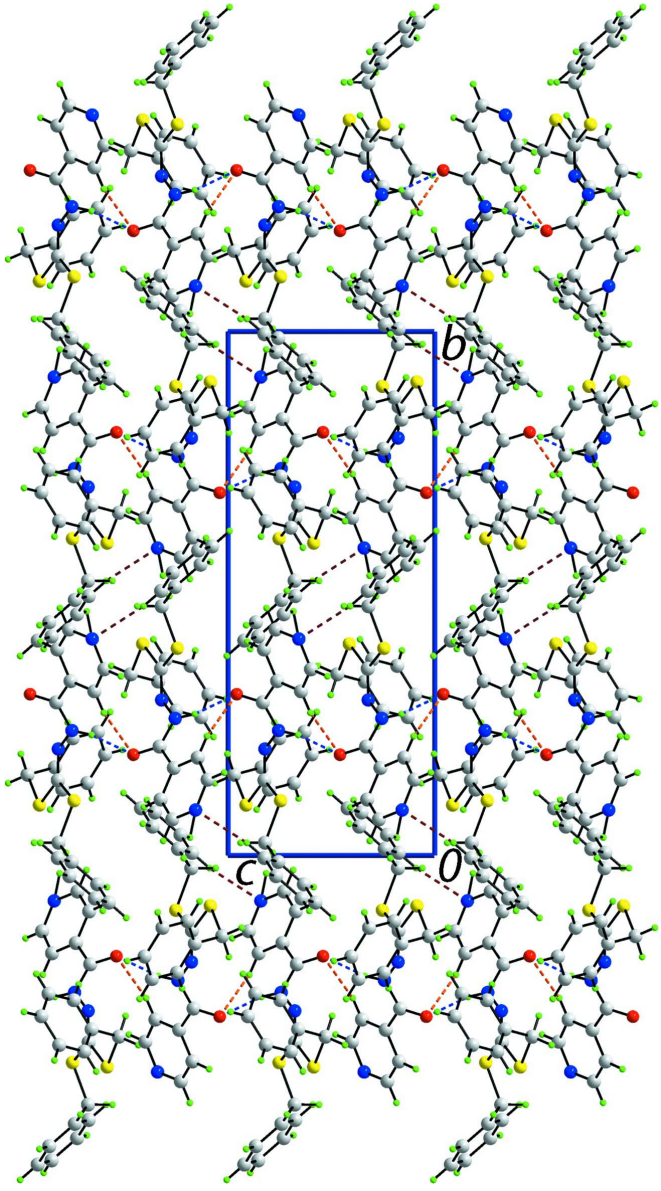

Figure 3

A view in projection down the *a* axis of the unit-cell contents for (I). The N—H···O, C—H···O and C—H···N interactions are shown as blue orange and brown dashed lines, respectively.

N′-[Bis(benzylsulfanyl)methylidene]benzohydrazide

Crystal data

$C_{21}H_{19}N_3OS_2$
M_r = 393.51
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.2593 (4) Å
b = 21.2182 (7) Å
c = 8.6041 (3) Å
β = 103.678 (3)°
V = 1997.24 (12) Å^3
Z = 4

$F(000) = 824$
$D_x = 1.309$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 17900 reflections
$\theta = 4–71°$
$\mu = 2.54$ mm^{-1}
$T = 150$ K
Block, dark yellow
0.50 × 0.36 × 0.16 mm

Data collection

Agilent Xcaliber Eos Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1952 pixels mm^{-1}
$\omega/2\theta$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
$T_{min} = 0.42$, $T_{max} = 0.67$
38338 measured reflections
3867 independent reflections
3715 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 71.4°$, $\theta_{min} = 4.0°$
$h = -13\rightarrow13$
$k = -24\rightarrow26$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.097$
$S = 1.03$
3867 reflections
247 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.6548P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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	0.58342 (3)	0.395419 (15)	0.24637 (4)	0.02644 (11)
S2	0.37808 (3)	0.403747 (16)	0.41378 (4)	0.03091 (12)
O1	0.55367 (12)	0.19229 (5)	0.45894 (12)	0.0423 (3)
N1	0.45622 (11)	0.29676 (5)	0.32219 (13)	0.0266 (2)
N2	0.53822 (10)	0.26152 (5)	0.25652 (13)	0.0246 (2)
H2N	0.5455 (15)	0.2700 (8)	0.161 (2)	0.030*
N3	0.82288 (13)	0.08675 (8)	0.1580 (2)	0.0510 (4)
C1	0.47186 (11)	0.35652 (7)	0.32465 (14)	0.0240 (3)
C2	0.58359 (14)	0.47567 (7)	0.32153 (18)	0.0316 (3)
H2A	0.5016	0.4948	0.2845	0.038*

H2B	0.6056	0.4758	0.4399	0.038*
C3	0.67684 (13)	0.51237 (7)	0.25762 (17)	0.0288 (3)
C4	0.64021 (15)	0.55501 (9)	0.1339 (2)	0.0423 (4)
H4	0.5556	0.5605	0.0867	0.051*
C5	0.72615 (19)	0.58997 (10)	0.0779 (2)	0.0525 (5)
H5	0.7001	0.6193	−0.0068	0.063*
C6	0.84883 (17)	0.58206 (9)	0.1453 (2)	0.0465 (4)
H6	0.9076	0.6057	0.1069	0.056*
C7	0.88623 (15)	0.53955 (8)	0.2688 (2)	0.0421 (4)
H7	0.9709	0.5341	0.3155	0.051*
C8	0.80055 (14)	0.50489 (7)	0.32481 (19)	0.0351 (3)
H8	0.8269	0.4758	0.4099	0.042*
C9	0.27606 (13)	0.34592 (7)	0.47123 (17)	0.0297 (3)
H9A	0.3219	0.3063	0.5034	0.036*
H9B	0.2487	0.3620	0.5651	0.036*
C10	0.16574 (13)	0.33186 (7)	0.33872 (17)	0.0308 (3)
C11	0.15710 (15)	0.27626 (9)	0.2525 (2)	0.0469 (4)
H11	0.2216	0.2463	0.2766	0.056*
C12	0.05412 (18)	0.26418 (11)	0.1306 (3)	0.0620 (6)
H12	0.0489	0.2261	0.0712	0.074*
C13	−0.04034 (18)	0.30698 (12)	0.0955 (2)	0.0582 (5)
H13	−0.1102	0.2986	0.0116	0.070*
C14	−0.03337 (18)	0.36186 (10)	0.1820 (2)	0.0555 (5)
H14	−0.0989	0.3912	0.1591	0.067*
C15	0.06947 (16)	0.37429 (8)	0.3028 (2)	0.0441 (4)
H15	0.0741	0.4124	0.3618	0.053*
C16	0.57822 (13)	0.20778 (6)	0.33232 (15)	0.0262 (3)
C17	0.66171 (12)	0.16710 (7)	0.26297 (16)	0.0277 (3)
C18	0.72075 (14)	0.18668 (8)	0.14762 (18)	0.0352 (3)
H18	0.7077	0.2277	0.1026	0.042*
C19	0.79978 (15)	0.14459 (10)	0.0994 (2)	0.0475 (4)
H19	0.8397	0.1581	0.0195	0.057*
C20	0.76652 (16)	0.06886 (9)	0.2706 (2)	0.0489 (4)
H20	0.7824	0.0278	0.3144	0.059*
C21	0.68633 (15)	0.10680 (7)	0.3272 (2)	0.0381 (4)
H21	0.6487	0.0921	0.4082	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02696 (19)	0.02388 (19)	0.03094 (19)	−0.00467 (12)	0.01177 (14)	−0.00630 (12)
S2	0.0295 (2)	0.02387 (19)	0.0439 (2)	−0.00234 (12)	0.01763 (16)	−0.00832 (13)
O1	0.0760 (9)	0.0293 (6)	0.0282 (5)	0.0116 (5)	0.0256 (5)	0.0044 (4)
N1	0.0300 (6)	0.0239 (6)	0.0292 (6)	0.0011 (4)	0.0134 (5)	−0.0024 (4)
N2	0.0309 (6)	0.0230 (6)	0.0232 (5)	0.0012 (4)	0.0129 (4)	−0.0005 (4)
N3	0.0308 (7)	0.0560 (10)	0.0626 (10)	0.0119 (7)	0.0037 (7)	−0.0243 (8)
C1	0.0233 (6)	0.0253 (7)	0.0238 (6)	−0.0008 (5)	0.0067 (5)	−0.0035 (5)
C2	0.0332 (7)	0.0232 (7)	0.0420 (8)	−0.0061 (5)	0.0159 (6)	−0.0090 (6)

C3	0.0312 (7)	0.0242 (7)	0.0328 (7)	−0.0057 (5)	0.0115 (6)	−0.0065 (5)
C4	0.0343 (8)	0.0482 (10)	0.0408 (8)	−0.0068 (7)	0.0017 (6)	0.0066 (7)
C5	0.0559 (11)	0.0585 (12)	0.0407 (9)	−0.0109 (9)	0.0067 (8)	0.0181 (8)
C6	0.0450 (9)	0.0502 (10)	0.0493 (9)	−0.0164 (8)	0.0213 (8)	0.0037 (8)
C7	0.0292 (8)	0.0413 (9)	0.0567 (10)	−0.0062 (7)	0.0123 (7)	0.0017 (7)
C8	0.0325 (8)	0.0301 (8)	0.0432 (8)	−0.0020 (6)	0.0096 (6)	0.0034 (6)
C9	0.0297 (7)	0.0292 (7)	0.0340 (7)	−0.0023 (5)	0.0153 (6)	−0.0026 (6)
C10	0.0312 (7)	0.0316 (7)	0.0339 (7)	−0.0053 (6)	0.0166 (6)	−0.0028 (6)
C11	0.0328 (8)	0.0466 (10)	0.0657 (11)	−0.0076 (7)	0.0207 (8)	−0.0230 (9)
C12	0.0445 (10)	0.0750 (14)	0.0714 (13)	−0.0194 (10)	0.0237 (9)	−0.0421 (11)
C13	0.0388 (10)	0.0868 (15)	0.0471 (10)	−0.0165 (10)	0.0069 (8)	−0.0133 (10)
C14	0.0430 (10)	0.0600 (12)	0.0576 (11)	0.0036 (9)	0.0004 (8)	0.0024 (9)
C15	0.0433 (9)	0.0379 (9)	0.0487 (9)	0.0024 (7)	0.0058 (7)	−0.0035 (7)
C16	0.0341 (7)	0.0230 (7)	0.0217 (6)	−0.0012 (5)	0.0071 (5)	−0.0037 (5)
C17	0.0261 (7)	0.0296 (7)	0.0246 (6)	0.0005 (5)	0.0006 (5)	−0.0084 (5)
C18	0.0296 (7)	0.0448 (9)	0.0314 (7)	0.0052 (6)	0.0073 (6)	−0.0037 (6)
C19	0.0301 (8)	0.0687 (12)	0.0451 (9)	0.0065 (8)	0.0116 (7)	−0.0148 (9)
C20	0.0382 (9)	0.0370 (9)	0.0662 (11)	0.0098 (7)	0.0018 (8)	−0.0138 (8)
C21	0.0374 (8)	0.0283 (8)	0.0465 (9)	0.0024 (6)	0.0059 (7)	−0.0062 (6)

Geometric parameters (Å, º)

S1—C1	1.7643 (13)	C8—H8	0.9500
S1—C2	1.8213 (14)	C9—C10	1.504 (2)
S2—C1	1.7579 (13)	C9—H9A	0.9900
S2—C9	1.8270 (14)	C9—H9B	0.9900
O1—C16	1.2304 (17)	C10—C11	1.385 (2)
N1—C1	1.2795 (18)	C10—C15	1.387 (2)
N1—N2	1.4063 (15)	C11—C12	1.391 (3)
N2—C16	1.3376 (18)	C11—H11	0.9500
N2—H2N	0.867 (18)	C12—C13	1.377 (3)
N3—C20	1.333 (3)	C12—H12	0.9500
N3—C19	1.329 (3)	C13—C14	1.374 (3)
C2—C3	1.5113 (19)	C13—H13	0.9500
C2—H2A	0.9900	C14—C15	1.386 (3)
C2—H2B	0.9900	C14—H14	0.9500
C3—C8	1.385 (2)	C15—H15	0.9500
C3—C4	1.384 (2)	C16—C17	1.5001 (18)
C4—C5	1.392 (2)	C17—C18	1.383 (2)
C4—H4	0.9500	C17—C21	1.395 (2)
C5—C6	1.376 (3)	C18—C19	1.391 (2)
C5—H5	0.9500	C18—H18	0.9500
C6—C7	1.382 (3)	C19—H19	0.9500
C6—H6	0.9500	C20—C21	1.381 (2)
C7—C8	1.387 (2)	C20—H20	0.9500
C7—H7	0.9500	C21—H21	0.9500
C1—S1—C2	104.06 (6)	S2—C9—H9B	109.0

C1—S2—C9	102.48 (7)	H9A—C9—H9B	107.8
C1—N1—N2	115.64 (11)	C11—C10—C15	118.79 (15)
C16—N2—N1	115.76 (11)	C11—C10—C9	121.06 (14)
C16—N2—H2N	123.0 (12)	C15—C10—C9	120.14 (14)
N1—N2—H2N	119.4 (11)	C10—C11—C12	120.09 (18)
C20—N3—C19	117.05 (15)	C10—C11—H11	120.0
N1—C1—S2	118.53 (10)	C12—C11—H11	120.0
N1—C1—S1	124.39 (10)	C13—C12—C11	120.47 (18)
S2—C1—S1	117.07 (8)	C13—C12—H12	119.8
C3—C2—S1	107.16 (9)	C11—C12—H12	119.8
C3—C2—H2A	110.3	C12—C13—C14	119.84 (18)
S1—C2—H2A	110.3	C12—C13—H13	120.1
C3—C2—H2B	110.3	C14—C13—H13	120.1
S1—C2—H2B	110.3	C13—C14—C15	119.87 (19)
H2A—C2—H2B	108.5	C13—C14—H14	120.1
C8—C3—C4	118.91 (14)	C15—C14—H14	120.1
C8—C3—C2	120.38 (13)	C14—C15—C10	120.92 (17)
C4—C3—C2	120.69 (13)	C14—C15—H15	119.5
C3—C4—C5	120.62 (16)	C10—C15—H15	119.5
C3—C4—H4	119.7	O1—C16—N2	122.64 (13)
C5—C4—H4	119.7	O1—C16—C17	119.44 (12)
C6—C5—C4	119.99 (16)	N2—C16—C17	117.84 (12)
C6—C5—H5	120.0	C18—C17—C21	118.39 (14)
C4—C5—H5	120.0	C18—C17—C16	124.44 (13)
C5—C6—C7	119.77 (15)	C21—C17—C16	117.05 (13)
C5—C6—H6	120.1	C17—C18—C19	118.11 (16)
C7—C6—H6	120.1	C17—C18—H18	120.9
C6—C7—C8	120.20 (16)	C19—C18—H18	120.9
C6—C7—H7	119.9	N3—C19—C18	124.13 (17)
C8—C7—H7	119.9	N3—C19—H19	117.9
C3—C8—C7	120.51 (15)	C18—C19—H19	117.9
C3—C8—H8	119.7	N3—C20—C21	123.60 (18)
C7—C8—H8	119.7	N3—C20—H20	118.2
C10—C9—S2	112.79 (10)	C21—C20—H20	118.2
C10—C9—H9A	109.0	C20—C21—C17	118.70 (17)
S2—C9—H9A	109.0	C20—C21—H21	120.7
C10—C9—H9B	109.0	C17—C21—H21	120.6

C1—N1—N2—C16	139.71 (13)	C9—C10—C11—C12	179.87 (16)
N2—N1—C1—S2	−176.89 (9)	C10—C11—C12—C13	−0.5 (3)
N2—N1—C1—S1	2.25 (17)	C11—C12—C13—C14	−0.5 (3)
C9—S2—C1—N1	−2.38 (12)	C12—C13—C14—C15	0.9 (3)
C9—S2—C1—S1	178.42 (7)	C13—C14—C15—C10	−0.4 (3)
C2—S1—C1—N1	−168.24 (12)	C11—C10—C15—C14	−0.6 (3)
C2—S1—C1—S2	10.91 (9)	C9—C10—C15—C14	−179.43 (16)
C1—S1—C2—C3	−179.46 (10)	N1—N2—C16—O1	−5.9 (2)
S1—C2—C3—C8	−76.56 (15)	N1—N2—C16—C17	177.46 (11)
S1—C2—C3—C4	105.00 (15)	O1—C16—C17—C18	−162.44 (15)

C8—C3—C4—C5	−0.1 (3)	N2—C16—C17—C18	14.3 (2)
C2—C3—C4—C5	178.34 (16)	O1—C16—C17—C21	13.6 (2)
C3—C4—C5—C6	0.3 (3)	N2—C16—C17—C21	−169.68 (13)
C4—C5—C6—C7	−0.3 (3)	C21—C17—C18—C19	1.3 (2)
C5—C6—C7—C8	0.1 (3)	C16—C17—C18—C19	177.25 (13)
C4—C3—C8—C7	−0.1 (2)	C20—N3—C19—C18	−0.4 (3)
C2—C3—C8—C7	−178.54 (14)	C17—C18—C19—N3	−0.5 (2)
C6—C7—C8—C3	0.1 (3)	C19—N3—C20—C21	0.4 (3)
C1—S2—C9—C10	−86.57 (11)	N3—C20—C21—C17	0.4 (3)
S2—C9—C10—C11	104.40 (15)	C18—C17—C21—C20	−1.3 (2)
S2—C9—C10—C15	−76.77 (16)	C16—C17—C21—C20	−177.54 (14)
C15—C10—C11—C12	1.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*N*···O1^{i}	0.864 (17)	1.936 (17)	2.7852 (15)	167.4 (16)
C7—H7···N3^{ii}	0.95	2.54	3.339 (2)	142
C8—H8···N3^{iii}	0.95	2.52	3.424 (2)	158
C18—H18···O1^{i}	0.95	2.53	3.365 (2)	147

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