IUCrData

ISSN 2414-3146

1-Benzyl-2-benzylsulfanyl-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one

Rachida Akrad,[a]* Joel T Mague,[b] Walid Guerrab,[a] Jamal Taoufik,[a] Mhamed Ansar[a] and Youssef Ramli[a]

[a]Laboratory of Medicinal Chemistry, Faculty of Medicine and Pharmacy, University Mohammed V, Rabat, Morocco, and [b]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: rakrad@yahoo.com

Received 5 January 2017
Accepted 8 January 2017

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

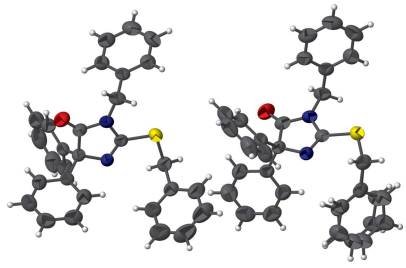
Keywords: crystal structure; imidazole; hydantoin; C-H···S hydrogen bonds; C—H···π interactions.

CCDC reference: 1526139

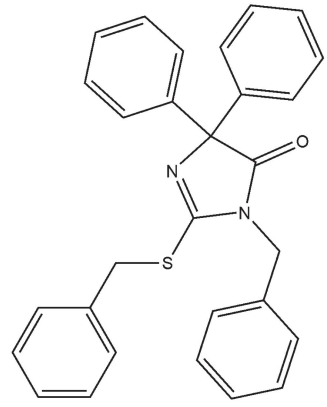
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{29}H_{24}N_2OS$, consists of two independent molecules having markedly different orientations of the substituents on the central imidazole ring. Apart from a weak C—H···S hydrogen bond, the intermolecular interactions in the crystal are all of the C—H···π(ring) type and form a three-dimensional network. One of the phenyl rings is disordered over two sets of sites in 0.713 (9): 0.287 (9) ratio.

3D view



Chemical scheme



Structure description

Hydantoin derivatives are known for their physiological activity as anticonvulsants (Weichet, 1974) and are also widely used in many other pharmacological applications such as antiarrhythmic (Havera *et al.*, 1976), antidiabetic (Rizzi *et al.*, 1989), fungicidal (Thenmozhiyal *et al.*, 2004), anti-carcinogen (Lamothe *et al.*, 2002), antiviral (el-Barbary *et al.*, 1994) and anti-HIV (Khodair *et al.*, 1997) agents.

The asymmetric unit of the title compound contains two independent molecules (*A* and *B*; Fig. 1). No part of one molecule is directly superimposable on the other, as shown by the AutoMolFit plot (Fig. 2), and the dihedral angles between the central five-membered imidazole rings and the peripheral benzene rings; see Table 1. The phenyl ring attached to atom C4 is rotationally disordered by 20.3 (2)° about the C4···C5*A*(or C5*B*) bond.

In the crystal, the two molecules are linked by a C—H···S hydrogen bond (Table 2). There are a number of C—H···π(ring) interactions present (Fig. 3 and Table 2), linking the molecules to form a three-dimensional network.

Table 1
Dihedral angles (°).

Ring 1	Ring 2	Dihedral angle
N1/N2/C1–C3	C5*A*–C10*A*	80.83 (16)
N1/N2/C1–C3	C12–C17	76.92 (11)
N1/N2/C1–C3	C18–C23	66.59 (11)
N1/N2/C1–C3	C24–C29	58.40 (11)
N3/N4/C30–C32	C34–C39	70.43 (12)
N3/N4/C30–C32	C41–C46	75.48 (10)
N3/N4/C30–C32	C47–C52	69.00 (10)
N3/N4/C30–C32	C53–C58	72.92 (11)

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

*Cg*2, *Cg*3, *Cg*5, *Cg*8 and *Cg*9 are the centroids of the C5*A*–C10*A*, C12–C17, C24–C29, C41–C46 and C47–C52 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···S2^{i}	0.97	2.95	3.591 (2)	125
C4—H4*B*···*Cg*8^{ii}	0.97	2.97	3.693 (2)	133
C11—H11*B*···*Cg*9^{i}	0.97	2.83	3.524 (2)	129
C22—H22···*Cg*8^{iii}	0.93	2.77	3.554 (3)	143
C35—H35···*Cg*5	0.93	2.77	3.697 (3)	172
C40—H40*A*···*Cg*3^{ii}	0.97	2.81	3.556 (2)	134
C55—H55···*Cg*2^{iv}	0.93	2.84	3.725 (3)	160

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

Synthesis and crystallization

To a solution of 5,5-diphenyl-2-thioxoimidazolidin-4-one (1.86 mol, 500.00 mg) in 10 ml DMF were added benzyl-chloride (3.73 mol), K_2CO_3 (3.73 mol) and a catalytic amount of tetrabutylammonium bromide. The mixture was stirred at room temperature for 24 h. The solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from ethanol solution to afford colourless block-like crystals of the title compound (yield 60%).

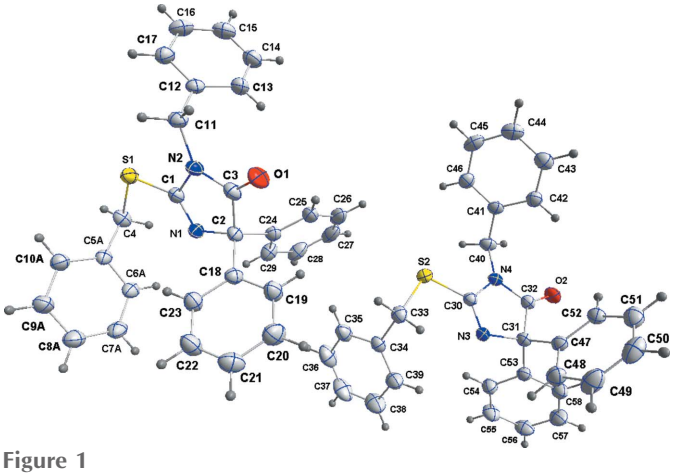


Figure 1
The molecular structure of the two independent molecules (molecule *A* left, molecule *B* right) of the title compound, with the atom labelling and 25% probability displacement ellipsoids. Only the major component (C5*A*–C10*A*) of the disordered phenyl ring is shown.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{24}N_2OS$
M_r	448.56
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	298
a, *b*, *c* (Å)	8.7383 (6), 14.1443 (9), 19.2405 (13)
α, β, γ (°)	90.732 (1), 92.181 (1), 91.394 (1)
V (Å^3)	2375.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.16
Crystal size (mm)	0.26 × 0.17 × 0.14
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.80, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22757, 11555, 6260
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.675
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.055, 0.158, 1.00
No. of reflections	11555
No. of parameters	590
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.17

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The phenyl ring attached to atom C4 of molecule A (Fig. 1) is disordered by a 20.3 (2)° rotation about the C4···C5*A*(or C5*B*) axis. The two components were

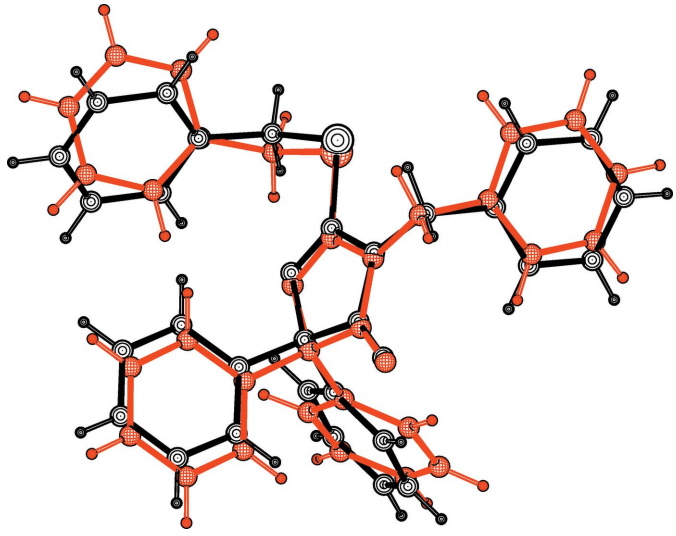


Figure 2
The AutoMolFit (*PLATON*; Spek, 2009) of molecule *B* (red) on molecule *A* (black); only the major component (C5*A*–C10*A*) of the disordered phenyl ring is shown.

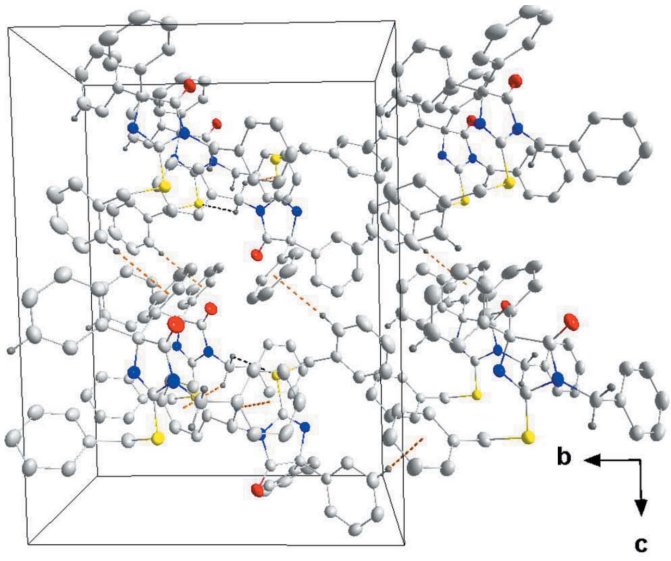


Figure 3
A view along the *a* axis of the crystal packing of the title compound. The C—H···S hydrogen bonds and C—H···π(ring) interactions are shown as, respectively, black and orange dotted lines (see Table 2; only the major component (C5*A*–C10*A*) of the disordered phenyl ring is shown).

refined as rigid hexagons with the displacement parameters of corresponding carbon atoms restrained to be comparable. The refined occupancy ratio (*A*:*B*) is = 0.713 (9): 0.287 (9).

Acknowledgements

JTM thanks Tulane University for support of the Tulane Crystallography Laboratory.

References

el-Barbary, A. A., Khodair, A. I., Pedersen, E. B. & Nielsen, C. (1994). *J. Med. Chem.* **37**, 73–77.
Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SADABS* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Havera, H. J. & Strycker, W. G. (1976). US Patent 3 904 909.
Khodair, A. I., el-Subbagh, H. I. & el-Emam, A. A. (1997). *Boll. Chim. Farm.* **136**, 561–567.
Lamothe, M., Lannuzel, M. & Perez, M. (2002). *J. Comb. Chem.* **4**, 73–78.
Rizzi, J. P., Schnur, R. C., Hutson, N. J., Kraus, K. G. & Kelbaugh, P. R. (1989). *J. Med. Chem.* **32**, 1208–1213.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Thenmozhiyal, J. C., Wong, P. T. H. & Chui, W.-K. (2004). *J. Med. Chem.* **47**, 1527–1535.
Weichet, B. L. (1974). *J. Czech. Patent*, **151**, 744–747.

full crystallographic data

IUCrData (2017). **2**, x170033 [https://doi.org/10.1107/S2414314617000335]

1-Benzyl-2-benzylsulfanyl-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one

Rachida Akrad, Joel T Mague, Walid Guerrab, Jamal Taoufik, Mhamed Ansar and Youssef Ramli

1-Benzyl-2-benzylsulfanyl-4,4-diphenyl-4,5-dihydro-1*H*-imidazol-5-one

Crystal data

$C_{29}H_{24}N_2OS$
M_r = 448.56
Triclinic, $P\overline{1}$
a = 8.7383 (6) Å
b = 14.1443 (9) Å
c = 19.2405 (13) Å
α = 90.732 (1)°
β = 92.181 (1)°
γ = 91.394 (1)°
V = 2375.4 (3) Å^3
Z = 4
$F(000)$ = 944
D_x = 1.254 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4999 reflections
θ = 2.5–24.0°
μ = 0.16 mm^{-1}
T = 298 K
Block, colourless
0.26 × 0.17 × 0.14 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.80, T_{max} = 0.98
22757 measured reflections
11555 independent reflections
6260 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 28.7°, θ_{min} = 1.1°
h = −11→11
k = −19→19
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.158
S = 1.00
11555 reflections
590 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
$w = 1/[\sigma^2(F_o^2) + (0.0667P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 30 sec/frame was used.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.93 - 0.97 Å). All were included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms. The phenyl ring attached to C4 is disordered by a 20.3 (2)° rotation about the C4···C5A(or B) axis. The two components of the disorder were refined as rigid hexagons with the displacement parameters of corresponding carbon atoms restrained to be comparable.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1	0.10005 (6)	0.34338 (4)	0.19831 (3)	0.05694 (16)	
O1	−0.07564 (18)	0.42328 (11)	0.43322 (8)	0.0769 (5)	
N1	0.14932 (18)	0.27553 (11)	0.32783 (8)	0.0502 (4)	
N2	−0.00086 (18)	0.40342 (10)	0.32105 (8)	0.0519 (4)	
C1	0.0883 (2)	0.33659 (13)	0.28826 (10)	0.0477 (4)	
C2	0.1037 (2)	0.29822 (13)	0.39949 (10)	0.0507 (5)	
C3	−0.0032 (2)	0.38249 (14)	0.39060 (11)	0.0557 (5)	
C4	0.2168 (2)	0.24238 (14)	0.18086 (11)	0.0629 (6)	
H4A	0.2529	0.2472	0.1340	0.075*	
H4B	0.3059	0.2451	0.2125	0.075*	
C5A	0.1368 (4)	0.1480 (2)	0.1879 (2)	0.0505 (6)	0.713 (9)
C6A	0.2058 (4)	0.0894 (3)	0.2367 (2)	0.0606 (10)	0.713 (9)
H6A	0.2925	0.1106	0.2624	0.073*	0.713 (9)
C7A	0.1451 (6)	−0.0008 (3)	0.24713 (16)	0.0715 (12)	0.713 (9)
H7A	0.1912	−0.0400	0.2798	0.086*	0.713 (9)
C8A	0.0155 (4)	−0.0325 (2)	0.2087 (3)	0.0828 (12)	0.713 (9)
H8A	−0.0251	−0.0929	0.2157	0.099*	0.713 (9)
C9A	−0.0534 (3)	0.0261 (2)	0.1599 (3)	0.0817 (14)	0.713 (9)
H9A	−0.1401	0.0049	0.1342	0.098*	0.713 (9)
C10A	0.0072 (5)	0.1163 (2)	0.1495 (2)	0.0663 (11)	0.713 (9)
H10A	−0.0389	0.1555	0.1169	0.080*	0.713 (9)
C5B	0.1503 (11)	0.1425 (7)	0.1908 (6)	0.0505 (6)	0.287 (9)
C6B	0.1623 (14)	0.0806 (9)	0.2461 (5)	0.0606 (10)	0.287 (9)
H6B	0.2234	0.0969	0.2852	0.073*	0.287 (9)
C7B	0.0829 (14)	−0.0058 (8)	0.2429 (5)	0.0715 (12)	0.287 (9)
H7B	0.0909	−0.0473	0.2799	0.086*	0.287 (9)
C8B	−0.0084 (12)	−0.0303 (6)	0.1844 (6)	0.0828 (12)	0.287 (9)
H8B	−0.0615	−0.0881	0.1823	0.099*	0.287 (9)
C9B	−0.0204 (13)	0.0317 (7)	0.1291 (6)	0.0817 (14)	0.287 (9)
H9B	−0.0815	0.0153	0.0899	0.098*	0.287 (9)

C10B	0.0590 (13)	0.1181 (7)	0.1323 (5)	0.0663 (11)	0.287 (9)
H10B	0.0510	0.1596	0.0952	0.080*	0.287 (9)
C11	−0.0818 (2)	0.48205 (13)	0.28914 (12)	0.0595 (5)	
H11A	−0.1650	0.4994	0.3183	0.071*	
H11B	−0.1263	0.4612	0.2444	0.071*	
C12	0.0194 (2)	0.56819 (13)	0.27865 (11)	0.0536 (5)	
C13	0.1074 (3)	0.60719 (14)	0.33321 (12)	0.0635 (6)	
H13	0.1054	0.5795	0.3768	0.076*	
C14	0.1979 (3)	0.68627 (16)	0.32411 (14)	0.0749 (7)	
H14	0.2576	0.7110	0.3614	0.090*	
C15	0.2014 (3)	0.72913 (17)	0.26111 (16)	0.0795 (7)	
H15	0.2625	0.7831	0.2554	0.095*	
C16	0.1147 (3)	0.69218 (18)	0.20651 (15)	0.0813 (7)	
H16	0.1164	0.7211	0.1634	0.098*	
C17	0.0234 (3)	0.61138 (16)	0.21486 (12)	0.0678 (6)	
H17	−0.0351	0.5864	0.1773	0.081*	
C18	0.0139 (2)	0.21601 (13)	0.43057 (10)	0.0529 (5)	
C19	−0.0179 (3)	0.21582 (17)	0.50014 (12)	0.0714 (6)	
H19	0.0170	0.2660	0.5286	0.086*	
C20	−0.1009 (3)	0.14228 (19)	0.52832 (14)	0.0830 (7)	
H20	−0.1213	0.1431	0.5754	0.100*	
C21	−0.1530 (3)	0.06838 (18)	0.48679 (15)	0.0819 (7)	
H21	−0.2083	0.0185	0.5056	0.098*	
C22	−0.1239 (3)	0.06809 (17)	0.41832 (14)	0.0825 (7)	
H22	−0.1597	0.0177	0.3902	0.099*	
C23	−0.0416 (3)	0.14148 (15)	0.38929 (12)	0.0674 (6)	
H23	−0.0237	0.1405	0.3420	0.081*	
C24	0.2489 (2)	0.32512 (14)	0.44394 (10)	0.0545 (5)	
C25	0.2496 (3)	0.39422 (15)	0.49521 (11)	0.0665 (6)	
H25	0.1605	0.4264	0.5038	0.080*	
C26	0.3823 (4)	0.41545 (19)	0.53367 (13)	0.0899 (9)	
H26	0.3817	0.4618	0.5684	0.108*	
C27	0.5133 (4)	0.3704 (2)	0.52195 (15)	0.0953 (10)	
H27	0.6023	0.3864	0.5479	0.114*	
C28	0.5149 (3)	0.3002 (2)	0.47116 (15)	0.0915 (9)	
H28	0.6045	0.2684	0.4632	0.110*	
C29	0.3822 (3)	0.27788 (18)	0.43224 (12)	0.0707 (6)	
H29	0.3828	0.2308	0.3981	0.085*	
S2	0.37902 (6)	0.34701 (4)	0.71215 (3)	0.05625 (16)	
O2	0.60094 (16)	0.40572 (10)	0.95067 (7)	0.0659 (4)	
N3	0.35844 (18)	0.26232 (10)	0.83655 (7)	0.0478 (4)	
N4	0.50878 (17)	0.39542 (10)	0.83677 (8)	0.0486 (4)	
C30	0.4122 (2)	0.32950 (12)	0.80067 (9)	0.0456 (4)	
C31	0.4139 (2)	0.28060 (12)	0.90933 (9)	0.0478 (4)	
C32	0.5216 (2)	0.36797 (13)	0.90528 (10)	0.0499 (5)	
C33	0.2558 (2)	0.24505 (14)	0.69060 (10)	0.0568 (5)	
H33A	0.1926	0.2315	0.7298	0.068*	
H33B	0.1882	0.2604	0.6514	0.068*	

C34	0.3414 (2)	0.15830 (14)	0.67276 (10)	0.0532 (5)
C35	0.4014 (3)	0.15061 (17)	0.60760 (13)	0.0771 (7)
H35	0.3852	0.1982	0.5754	0.093*
C36	0.4842 (3)	0.0741 (2)	0.58992 (17)	0.1015 (10)
H36	0.5252	0.0703	0.5461	0.122*
C37	0.5071 (4)	0.0035 (2)	0.6358 (2)	0.1095 (11)
H37	0.5638	−0.0485	0.6234	0.131*
C38	0.4469 (4)	0.0087 (2)	0.70049 (18)	0.1054 (10)
H38	0.4614	−0.0402	0.7318	0.126*
C39	0.3639 (3)	0.08743 (16)	0.71928 (13)	0.0722 (6)
H39	0.3240	0.0916	0.7633	0.087*
C40	0.5916 (2)	0.47636 (13)	0.80867 (11)	0.0571 (5)
H40A	0.6353	0.4574	0.7652	0.068*
H40B	0.6756	0.4946	0.8409	0.068*
C41	0.4928 (2)	0.56105 (13)	0.79590 (10)	0.0497 (5)
C42	0.4154 (2)	0.60108 (14)	0.84996 (11)	0.0577 (5)
H42	0.4223	0.5749	0.8940	0.069*
C43	0.3283 (2)	0.67962 (16)	0.83860 (12)	0.0667 (6)
H43	0.2763	0.7058	0.8752	0.080*
C44	0.3170 (3)	0.71991 (16)	0.77418 (14)	0.0707 (6)
H44	0.2579	0.7729	0.7669	0.085*
C45	0.3940 (3)	0.68097 (17)	0.72096 (13)	0.0714 (6)
H45	0.3878	0.7080	0.6772	0.086*
C46	0.4814 (2)	0.60162 (15)	0.73131 (11)	0.0610 (5)
H46	0.5327	0.5756	0.6944	0.073*
C47	0.2719 (2)	0.30247 (13)	0.95070 (9)	0.0490 (5)
C48	0.1514 (3)	0.23789 (17)	0.94676 (11)	0.0712 (6)
H48	0.1609	0.1808	0.9230	0.085*
C49	0.0147 (3)	0.2586 (2)	0.97858 (13)	0.0858 (8)
H49	−0.0675	0.2156	0.9752	0.103*
C50	0.0016 (3)	0.3416 (2)	1.01452 (13)	0.0837 (8)
H50	−0.0899	0.3555	1.0351	0.100*
C51	0.1231 (3)	0.40426 (18)	1.02018 (12)	0.0739 (7)
H51	0.1146	0.4601	1.0456	0.089*
C52	0.2580 (2)	0.38532 (14)	0.98854 (10)	0.0579 (5)
H52	0.3400	0.4284	0.9927	0.070*
C53	0.5052 (2)	0.19834 (13)	0.93806 (10)	0.0502 (5)
C54	0.5734 (2)	0.13524 (15)	0.89392 (11)	0.0652 (6)
H54	0.5594	0.1413	0.8460	0.078*
C55	0.6617 (3)	0.06354 (17)	0.92016 (14)	0.0786 (7)
H55	0.7061	0.0214	0.8899	0.094*
C56	0.6842 (3)	0.05415 (17)	0.99051 (14)	0.0779 (7)
H56	0.7438	0.0058	1.0082	0.093*
C57	0.6184 (3)	0.11649 (18)	1.03456 (13)	0.0774 (7)
H57	0.6340	0.1105	1.0824	0.093*
C58	0.5293 (3)	0.18795 (15)	1.00898 (11)	0.0664 (6)
H58	0.4849	0.2296	1.0396	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0650 (3)	0.0517 (3)	0.0544 (3)	0.0022 (3)	0.0049 (2)	0.0039 (2)
O1	0.0881 (11)	0.0683 (10)	0.0761 (10)	0.0265 (9)	0.0185 (9)	−0.0159 (8)
N1	0.0554 (10)	0.0458 (9)	0.0500 (9)	0.0096 (8)	0.0050 (8)	−0.0027 (7)
N2	0.0538 (10)	0.0411 (9)	0.0612 (10)	0.0098 (7)	0.0028 (8)	−0.0018 (8)
C1	0.0465 (11)	0.0415 (10)	0.0548 (11)	0.0012 (9)	0.0018 (9)	−0.0032 (9)
C2	0.0570 (12)	0.0447 (11)	0.0507 (11)	0.0085 (9)	0.0043 (9)	−0.0059 (9)
C3	0.0560 (12)	0.0462 (11)	0.0650 (14)	0.0067 (10)	0.0048 (10)	−0.0091 (10)
C4	0.0613 (13)	0.0626 (13)	0.0656 (13)	0.0007 (11)	0.0164 (11)	−0.0072 (11)
C5A	0.0517 (13)	0.0496 (12)	0.0506 (12)	0.0127 (11)	0.0016 (10)	−0.0045 (10)
C6A	0.070 (3)	0.0546 (17)	0.0581 (17)	0.0146 (19)	0.0051 (19)	−0.0030 (14)
C7A	0.076 (4)	0.0615 (18)	0.0778 (19)	0.019 (2)	−0.003 (2)	0.0074 (14)
C8A	0.088 (2)	0.0642 (17)	0.096 (4)	−0.0002 (16)	−0.004 (3)	0.016 (2)
C9A	0.078 (2)	0.0668 (18)	0.098 (4)	−0.0157 (18)	−0.017 (2)	0.018 (3)
C10A	0.060 (3)	0.0620 (15)	0.076 (3)	−0.0030 (19)	−0.006 (2)	0.0127 (16)
C5B	0.0517 (13)	0.0496 (12)	0.0506 (12)	0.0127 (11)	0.0016 (10)	−0.0045 (10)
C6B	0.070 (3)	0.0546 (17)	0.0581 (17)	0.0146 (19)	0.0051 (19)	−0.0030 (14)
C7B	0.076 (4)	0.0615 (18)	0.0778 (19)	0.019 (2)	−0.003 (2)	0.0074 (14)
C8B	0.088 (2)	0.0642 (17)	0.096 (4)	−0.0002 (16)	−0.004 (3)	0.016 (2)
C9B	0.078 (2)	0.0668 (18)	0.098 (4)	−0.0157 (18)	−0.017 (2)	0.018 (3)
C10B	0.060 (3)	0.0620 (15)	0.076 (3)	−0.0030 (19)	−0.006 (2)	0.0127 (16)
C11	0.0531 (12)	0.0452 (11)	0.0798 (15)	0.0125 (10)	−0.0102 (10)	0.0023 (10)
C12	0.0528 (12)	0.0447 (11)	0.0640 (13)	0.0167 (9)	0.0000 (10)	0.0003 (10)
C13	0.0717 (14)	0.0507 (12)	0.0677 (14)	0.0040 (11)	−0.0039 (11)	0.0015 (10)
C14	0.0740 (16)	0.0568 (14)	0.0931 (18)	0.0006 (12)	−0.0050 (13)	−0.0073 (13)
C15	0.0740 (17)	0.0512 (13)	0.114 (2)	0.0073 (12)	0.0099 (16)	0.0089 (14)
C16	0.0870 (18)	0.0704 (16)	0.0893 (18)	0.0236 (15)	0.0164 (15)	0.0293 (14)
C17	0.0700 (15)	0.0652 (14)	0.0686 (14)	0.0194 (12)	−0.0045 (12)	0.0049 (12)
C18	0.0548 (12)	0.0468 (11)	0.0578 (12)	0.0078 (10)	0.0058 (10)	0.0002 (9)
C19	0.0827 (16)	0.0674 (14)	0.0642 (14)	−0.0096 (13)	0.0153 (12)	−0.0070 (11)
C20	0.0876 (18)	0.0861 (18)	0.0766 (16)	−0.0065 (15)	0.0232 (14)	0.0066 (14)
C21	0.0756 (17)	0.0683 (16)	0.103 (2)	−0.0088 (13)	0.0200 (15)	0.0084 (15)
C22	0.0854 (18)	0.0687 (16)	0.0922 (19)	−0.0209 (14)	0.0050 (15)	−0.0119 (14)
C23	0.0690 (14)	0.0654 (14)	0.0672 (14)	−0.0074 (12)	0.0024 (11)	−0.0058 (11)
C24	0.0595 (13)	0.0520 (12)	0.0520 (12)	−0.0041 (10)	0.0020 (10)	0.0061 (9)
C25	0.0859 (16)	0.0556 (13)	0.0569 (13)	−0.0109 (12)	−0.0046 (12)	0.0010 (10)
C26	0.124 (2)	0.0737 (17)	0.0683 (16)	−0.0311 (18)	−0.0228 (17)	0.0164 (13)
C27	0.096 (2)	0.107 (2)	0.0788 (19)	−0.0389 (19)	−0.0321 (17)	0.0371 (17)
C28	0.0670 (16)	0.127 (2)	0.0813 (18)	0.0023 (17)	−0.0053 (14)	0.0386 (18)
C29	0.0640 (14)	0.0871 (17)	0.0616 (14)	0.0094 (13)	0.0022 (11)	0.0114 (12)
S2	0.0694 (4)	0.0486 (3)	0.0510 (3)	0.0041 (2)	0.0011 (2)	0.0068 (2)
O2	0.0669 (9)	0.0606 (9)	0.0683 (9)	−0.0139 (8)	−0.0090 (8)	−0.0109 (7)
N3	0.0575 (10)	0.0421 (8)	0.0437 (9)	−0.0031 (7)	0.0015 (7)	−0.0006 (7)
N4	0.0506 (9)	0.0396 (8)	0.0555 (10)	−0.0020 (7)	0.0026 (7)	0.0009 (7)
C30	0.0482 (11)	0.0396 (10)	0.0493 (11)	0.0039 (9)	0.0047 (8)	−0.0011 (8)
C31	0.0532 (11)	0.0431 (10)	0.0467 (11)	−0.0039 (9)	0.0013 (9)	−0.0010 (8)

C32	0.0509 (11)	0.0444 (11)	0.0542 (12)	0.0005 (9)	0.0040 (9)	−0.0051 (9)
C33	0.0541 (12)	0.0597 (13)	0.0560 (12)	0.0061 (10)	−0.0063 (9)	−0.0027 (10)
C34	0.0469 (11)	0.0542 (12)	0.0582 (12)	−0.0035 (9)	0.0028 (9)	−0.0078 (10)
C35	0.0855 (17)	0.0692 (15)	0.0772 (16)	−0.0111 (14)	0.0238 (13)	−0.0150 (13)
C36	0.088 (2)	0.106 (2)	0.111 (2)	−0.0009 (18)	0.0309 (18)	−0.041 (2)
C37	0.100 (2)	0.091 (2)	0.137 (3)	0.0375 (19)	−0.008 (2)	−0.041 (2)
C38	0.122 (2)	0.0768 (19)	0.116 (3)	0.0307 (18)	−0.033 (2)	−0.0021 (18)
C39	0.0792 (16)	0.0636 (14)	0.0731 (15)	0.0079 (13)	−0.0114 (12)	−0.0008 (12)
C40	0.0497 (11)	0.0466 (11)	0.0755 (14)	−0.0034 (9)	0.0115 (10)	0.0038 (10)
C41	0.0471 (11)	0.0415 (10)	0.0603 (12)	−0.0075 (9)	0.0056 (9)	0.0034 (9)
C42	0.0607 (13)	0.0537 (12)	0.0591 (12)	0.0002 (10)	0.0069 (10)	0.0002 (10)
C43	0.0623 (14)	0.0598 (13)	0.0786 (16)	0.0023 (11)	0.0108 (12)	−0.0074 (12)
C44	0.0609 (14)	0.0539 (13)	0.0977 (18)	0.0027 (11)	0.0035 (13)	0.0098 (13)
C45	0.0710 (15)	0.0697 (15)	0.0737 (15)	−0.0044 (13)	0.0007 (12)	0.0254 (13)
C46	0.0613 (13)	0.0589 (13)	0.0636 (13)	−0.0052 (11)	0.0143 (10)	0.0038 (11)
C47	0.0534 (11)	0.0494 (11)	0.0440 (11)	−0.0016 (9)	−0.0018 (9)	0.0052 (9)
C48	0.0727 (15)	0.0759 (16)	0.0646 (14)	−0.0149 (13)	0.0096 (12)	−0.0028 (12)
C49	0.0671 (16)	0.120 (2)	0.0697 (16)	−0.0258 (16)	0.0086 (13)	0.0112 (16)
C50	0.0663 (16)	0.124 (2)	0.0627 (15)	0.0194 (17)	0.0150 (12)	0.0208 (16)
C51	0.0794 (17)	0.0801 (17)	0.0639 (15)	0.0206 (14)	0.0109 (13)	0.0046 (12)
C52	0.0618 (13)	0.0552 (12)	0.0572 (12)	0.0073 (10)	0.0034 (10)	0.0026 (10)
C53	0.0537 (12)	0.0440 (10)	0.0525 (12)	−0.0030 (9)	−0.0009 (9)	0.0012 (9)
C54	0.0740 (15)	0.0627 (14)	0.0595 (13)	0.0089 (12)	0.0050 (11)	−0.0009 (11)
C55	0.0828 (17)	0.0650 (15)	0.0891 (19)	0.0245 (13)	0.0041 (14)	−0.0049 (13)
C56	0.0765 (16)	0.0628 (15)	0.0938 (19)	0.0127 (13)	−0.0131 (14)	0.0096 (14)
C57	0.0881 (17)	0.0768 (16)	0.0665 (15)	0.0100 (14)	−0.0151 (13)	0.0134 (13)
C58	0.0787 (15)	0.0629 (14)	0.0571 (13)	0.0083 (12)	−0.0055 (11)	−0.0019 (11)

Geometric parameters (Å, º)

S1—C1	1.7414 (19)	C26—H26	0.9300
S1—C4	1.811 (2)	C27—C28	1.385 (4)
O1—C3	1.205 (2)	C27—H27	0.9300
N1—C1	1.272 (2)	C28—C29	1.384 (3)
N1—C2	1.483 (2)	C28—H28	0.9300
N2—C3	1.375 (2)	C29—H29	0.9300
N2—C1	1.399 (2)	S2—C30	1.7386 (19)
N2—C11	1.462 (2)	S2—C33	1.813 (2)
C2—C18	1.528 (3)	O2—C32	1.205 (2)
C2—C3	1.539 (3)	N3—C30	1.273 (2)
C2—C24	1.540 (3)	N3—C31	1.482 (2)
C4—C5A	1.502 (3)	N4—C32	1.380 (2)
C4—C5B	1.531 (8)	N4—C30	1.402 (2)
C4—H4A	0.9700	N4—C40	1.460 (2)
C4—H4B	0.9700	C31—C53	1.524 (3)
C5A—C6A	1.3900	C31—C47	1.535 (3)
C5A—C10A	1.3900	C31—C32	1.540 (3)
C6A—C7A	1.3900	C33—C34	1.495 (3)

C6A—H6A	0.9300	C33—H33A	0.9700
C7A—C8A	1.3900	C33—H33B	0.9700
C7A—H7A	0.9300	C34—C39	1.365 (3)
C8A—C9A	1.3900	C34—C35	1.381 (3)
C8A—H8A	0.9300	C35—C36	1.363 (4)
C9A—C10A	1.3900	C35—H35	0.9300
C9A—H9A	0.9300	C36—C37	1.355 (4)
C10A—H10A	0.9300	C36—H36	0.9300
C5B—C6B	1.3900	C37—C38	1.371 (4)
C5B—C10B	1.3900	C37—H37	0.9300
C6B—C7B	1.3900	C38—C39	1.395 (4)
C6B—H6B	0.9300	C38—H38	0.9300
C7B—C8B	1.3900	C39—H39	0.9300
C7B—H7B	0.9300	C40—C41	1.511 (3)
C8B—C9B	1.3900	C40—H40A	0.9700
C8B—H8B	0.9300	C40—H40B	0.9700
C9B—C10B	1.3900	C41—C46	1.377 (3)
C9B—H9B	0.9300	C41—C42	1.385 (3)
C10B—H10B	0.9300	C42—C43	1.377 (3)
C11—C12	1.508 (3)	C42—H42	0.9300
C11—H11A	0.9700	C43—C44	1.372 (3)
C11—H11B	0.9700	C43—H43	0.9300
C12—C13	1.379 (3)	C44—C45	1.364 (3)
C12—C17	1.379 (3)	C44—H44	0.9300
C13—C14	1.371 (3)	C45—C46	1.385 (3)
C13—H13	0.9300	C45—H45	0.9300
C14—C15	1.363 (3)	C46—H46	0.9300
C14—H14	0.9300	C47—C48	1.376 (3)
C15—C16	1.363 (3)	C47—C52	1.382 (3)
C15—H15	0.9300	C48—C49	1.398 (3)
C16—C17	1.392 (3)	C48—H48	0.9300
C16—H16	0.9300	C49—C50	1.365 (4)
C17—H17	0.9300	C49—H49	0.9300
C18—C19	1.377 (3)	C50—C51	1.366 (4)
C18—C23	1.379 (3)	C50—H50	0.9300
C19—C20	1.382 (3)	C51—C52	1.378 (3)
C19—H19	0.9300	C51—H51	0.9300
C20—C21	1.366 (3)	C52—H52	0.9300
C20—H20	0.9300	C53—C58	1.383 (3)
C21—C22	1.351 (3)	C53—C54	1.385 (3)
C21—H21	0.9300	C54—C55	1.379 (3)
C22—C23	1.384 (3)	C54—H54	0.9300
C22—H22	0.9300	C55—C56	1.369 (3)
C23—H23	0.9300	C55—H55	0.9300
C24—C25	1.379 (3)	C56—C57	1.367 (3)
C24—C29	1.381 (3)	C56—H56	0.9300
C25—C26	1.377 (3)	C57—C58	1.376 (3)
C25—H25	0.9300	C57—H57	0.9300

C26—C27	1.348 (4)	C58—H58	0.9300
C1—S1—C4	100.73 (10)	C26—C27—C28	119.8 (3)
C1—N1—C2	106.73 (15)	C26—C27—H27	120.1
C3—N2—C1	108.21 (15)	C28—C27—H27	120.1
C3—N2—C11	124.11 (16)	C29—C28—C27	119.6 (3)
C1—N2—C11	127.67 (17)	C29—C28—H28	120.2
N1—C1—N2	115.74 (17)	C27—C28—H28	120.2
N1—C1—S1	126.99 (15)	C24—C29—C28	120.3 (2)
N2—C1—S1	117.24 (14)	C24—C29—H29	119.9
N1—C2—C18	111.41 (15)	C28—C29—H29	119.9
N1—C2—C3	104.30 (15)	C30—S2—C33	100.11 (9)
C18—C2—C3	108.69 (15)	C30—N3—C31	106.47 (15)
N1—C2—C24	108.53 (15)	C32—N4—C30	107.94 (15)
C18—C2—C24	111.90 (15)	C32—N4—C40	124.05 (16)
C3—C2—C24	111.78 (15)	C30—N4—C40	127.90 (16)
O1—C3—N2	125.46 (19)	N3—C30—N4	116.01 (16)
O1—C3—C2	129.7 (2)	N3—C30—S2	126.77 (14)
N2—C3—C2	104.85 (16)	N4—C30—S2	117.22 (13)
C5A—C4—S1	114.8 (2)	N3—C31—C53	111.69 (14)
C5B—C4—S1	119.4 (4)	N3—C31—C47	106.37 (15)
C5A—C4—H4A	108.6	C53—C31—C47	113.66 (15)
S1—C4—H4A	108.6	N3—C31—C32	104.60 (14)
C5A—C4—H4B	108.6	C53—C31—C32	108.77 (15)
S1—C4—H4B	108.6	C47—C31—C32	111.38 (15)
H4A—C4—H4B	107.5	O2—C32—N4	126.24 (18)
C6A—C5A—C10A	120.0	O2—C32—C31	129.04 (18)
C6A—C5A—C4	114.3 (3)	N4—C32—C31	104.72 (15)
C10A—C5A—C4	125.7 (3)	C34—C33—S2	113.61 (14)
C7A—C6A—C5A	120.0	C34—C33—H33A	108.8
C7A—C6A—H6A	120.0	S2—C33—H33A	108.8
C5A—C6A—H6A	120.0	C34—C33—H33B	108.8
C6A—C7A—C8A	120.0	S2—C33—H33B	108.8
C6A—C7A—H7A	120.0	H33A—C33—H33B	107.7
C8A—C7A—H7A	120.0	C39—C34—C35	119.2 (2)
C9A—C8A—C7A	120.0	C39—C34—C33	121.96 (19)
C9A—C8A—H8A	120.0	C35—C34—C33	118.8 (2)
C7A—C8A—H8A	120.0	C36—C35—C34	120.8 (3)
C8A—C9A—C10A	120.0	C36—C35—H35	119.6
C8A—C9A—H9A	120.0	C34—C35—H35	119.6
C10A—C9A—H9A	120.0	C37—C36—C35	120.4 (3)
C9A—C10A—C5A	120.0	C37—C36—H36	119.8
C9A—C10A—H10A	120.0	C35—C36—H36	119.8
C5A—C10A—H10A	120.0	C36—C37—C38	120.1 (3)
C6B—C5B—C10B	120.0	C36—C37—H37	120.0
C6B—C5B—C4	131.7 (7)	C38—C37—H37	120.0
C10B—C5B—C4	108.2 (7)	C37—C38—C39	119.9 (3)
C5B—C6B—C7B	120.0	C37—C38—H38	120.1

C5B—C6B—H6B	120.0	C39—C38—H38	120.1
C7B—C6B—H6B	120.0	C34—C39—C38	119.7 (2)
C6B—C7B—C8B	120.0	C34—C39—H39	120.1
C6B—C7B—H7B	120.0	C38—C39—H39	120.1
C8B—C7B—H7B	120.0	N4—C40—C41	113.60 (15)
C9B—C8B—C7B	120.0	N4—C40—H40A	108.8
C9B—C8B—H8B	120.0	C41—C40—H40A	108.8
C7B—C8B—H8B	120.0	N4—C40—H40B	108.8
C8B—C9B—C10B	120.0	C41—C40—H40B	108.8
C8B—C9B—H9B	120.0	H40A—C40—H40B	107.7
C10B—C9B—H9B	120.0	C46—C41—C42	118.73 (19)
C9B—C10B—C5B	120.0	C46—C41—C40	121.05 (18)
C9B—C10B—H10B	120.0	C42—C41—C40	120.19 (18)
C5B—C10B—H10B	120.0	C43—C42—C41	120.1 (2)
N2—C11—C12	113.47 (15)	C43—C42—H42	119.9
N2—C11—H11A	108.9	C41—C42—H42	119.9
C12—C11—H11A	108.9	C44—C43—C42	121.1 (2)
N2—C11—H11B	108.9	C44—C43—H43	119.5
C12—C11—H11B	108.9	C42—C43—H43	119.5
H11A—C11—H11B	107.7	C45—C44—C43	118.9 (2)
C13—C12—C17	118.3 (2)	C45—C44—H44	120.5
C13—C12—C11	120.70 (19)	C43—C44—H44	120.5
C17—C12—C11	120.98 (19)	C44—C45—C46	120.8 (2)
C14—C13—C12	120.9 (2)	C44—C45—H45	119.6
C14—C13—H13	119.6	C46—C45—H45	119.6
C12—C13—H13	119.6	C41—C46—C45	120.3 (2)
C15—C14—C13	120.8 (2)	C41—C46—H46	119.8
C15—C14—H14	119.6	C45—C46—H46	119.8
C13—C14—H14	119.6	C48—C47—C52	119.34 (19)
C16—C15—C14	119.3 (2)	C48—C47—C31	117.69 (18)
C16—C15—H15	120.3	C52—C47—C31	122.90 (18)
C14—C15—H15	120.3	C47—C48—C49	119.7 (2)
C15—C16—C17	120.4 (2)	C47—C48—H48	120.2
C15—C16—H16	119.8	C49—C48—H48	120.2
C17—C16—H16	119.8	C50—C49—C48	120.3 (2)
C12—C17—C16	120.2 (2)	C50—C49—H49	119.9
C12—C17—H17	119.9	C48—C49—H49	119.9
C16—C17—H17	119.9	C49—C50—C51	119.9 (2)
C19—C18—C23	118.23 (19)	C49—C50—H50	120.1
C19—C18—C2	120.87 (18)	C51—C50—H50	120.1
C23—C18—C2	120.86 (18)	C50—C51—C52	120.5 (2)
C18—C19—C20	121.1 (2)	C50—C51—H51	119.7
C18—C19—H19	119.4	C52—C51—H51	119.7
C20—C19—H19	119.4	C51—C52—C47	120.2 (2)
C21—C20—C19	119.8 (2)	C51—C52—H52	119.9
C21—C20—H20	120.1	C47—C52—H52	119.9
C19—C20—H20	120.1	C58—C53—C54	118.22 (19)
C22—C21—C20	119.7 (2)	C58—C53—C31	120.74 (17)

C22—C21—H21	120.1	C54—C53—C31	120.94 (17)
C20—C21—H21	120.1	C55—C54—C53	120.7 (2)
C21—C22—C23	121.1 (2)	C55—C54—H54	119.6
C21—C22—H22	119.4	C53—C54—H54	119.6
C23—C22—H22	119.4	C56—C55—C54	120.3 (2)
C18—C23—C22	120.0 (2)	C56—C55—H55	119.8
C18—C23—H23	120.0	C54—C55—H55	119.8
C22—C23—H23	120.0	C57—C56—C55	119.4 (2)
C25—C24—C29	119.2 (2)	C57—C56—H56	120.3
C25—C24—C2	122.1 (2)	C55—C56—H56	120.3
C29—C24—C2	118.72 (19)	C56—C57—C58	120.8 (2)
C26—C25—C24	119.9 (3)	C56—C57—H57	119.6
C26—C25—H25	120.1	C58—C57—H57	119.6
C24—C25—H25	120.1	C57—C58—C53	120.5 (2)
C27—C26—C25	121.3 (3)	C57—C58—H58	119.7
C27—C26—H26	119.4	C53—C58—H58	119.7
C25—C26—H26	119.4		

C2—N1—C1—N2	−0.7 (2)	C25—C26—C27—C28	−1.1 (4)
C2—N1—C1—S1	−178.81 (14)	C26—C27—C28—C29	0.8 (4)
C3—N2—C1—N1	−2.0 (2)	C25—C24—C29—C28	−0.5 (3)
C11—N2—C1—N1	178.89 (17)	C2—C24—C29—C28	179.9 (2)
C3—N2—C1—S1	176.27 (13)	C27—C28—C29—C24	0.0 (4)
C11—N2—C1—S1	−2.8 (2)	C31—N3—C30—N4	2.8 (2)
C4—S1—C1—N1	0.5 (2)	C31—N3—C30—S2	−177.60 (14)
C4—S1—C1—N2	−177.61 (14)	C32—N4—C30—N3	0.5 (2)
C1—N1—C2—C18	119.89 (17)	C40—N4—C30—N3	176.89 (16)
C1—N1—C2—C3	2.81 (19)	C32—N4—C30—S2	−179.09 (13)
C1—N1—C2—C24	−116.48 (17)	C40—N4—C30—S2	−2.7 (2)
C1—N2—C3—O1	−176.15 (19)	C33—S2—C30—N3	−0.84 (19)
C11—N2—C3—O1	3.0 (3)	C33—S2—C30—N4	178.71 (13)
C1—N2—C3—C2	3.60 (19)	C30—N3—C31—C53	−122.17 (16)
C11—N2—C3—C2	−177.29 (16)	C30—N3—C31—C47	113.29 (17)
N1—C2—C3—O1	175.8 (2)	C30—N3—C31—C32	−4.69 (19)
C18—C2—C3—O1	56.9 (3)	C30—N4—C32—O2	176.50 (18)
C24—C2—C3—O1	−67.1 (3)	C40—N4—C32—O2	0.0 (3)
N1—C2—C3—N2	−3.92 (19)	C30—N4—C32—C31	−3.46 (19)
C18—C2—C3—N2	−122.86 (17)	C40—N4—C32—C31	179.99 (15)
C24—C2—C3—N2	113.14 (17)	N3—C31—C32—O2	−175.02 (19)
C1—S1—C4—C5A	72.3 (2)	C53—C31—C32—O2	−55.6 (3)
C1—S1—C4—C5B	68.6 (5)	C47—C31—C32—O2	70.5 (3)
S1—C4—C5A—C6A	−121.1 (2)	N3—C31—C32—N4	4.94 (19)
S1—C4—C5A—C10A	60.5 (4)	C53—C31—C32—N4	124.40 (16)
C10A—C5A—C6A—C7A	0.0	C47—C31—C32—N4	−109.57 (17)
C4—C5A—C6A—C7A	−178.5 (3)	C30—S2—C33—C34	−87.24 (16)
C5A—C6A—C7A—C8A	0.0	S2—C33—C34—C39	101.1 (2)
C6A—C7A—C8A—C9A	0.0	S2—C33—C34—C35	−77.9 (2)
C7A—C8A—C9A—C10A	0.0	C39—C34—C35—C36	−1.0 (3)

C8A—C9A—C10A—C5A	0.0	C33—C34—C35—C36	178.0 (2)
C6A—C5A—C10A—C9A	0.0	C34—C35—C36—C37	0.9 (4)
C4—C5A—C10A—C9A	178.3 (4)	C35—C36—C37—C38	0.0 (5)
S1—C4—C5B—C6B	−96.4 (7)	C36—C37—C38—C39	−0.9 (5)
S1—C4—C5B—C10B	80.7 (7)	C35—C34—C39—C38	0.1 (3)
C10B—C5B—C6B—C7B	0.0	C33—C34—C39—C38	−178.9 (2)
C4—C5B—C6B—C7B	176.8 (10)	C37—C38—C39—C34	0.9 (4)
C5B—C6B—C7B—C8B	0.0	C32—N4—C40—C41	−104.9 (2)
C6B—C7B—C8B—C9B	0.0	C30—N4—C40—C41	79.3 (2)
C7B—C8B—C9B—C10B	0.0	N4—C40—C41—C46	−124.3 (2)
C8B—C9B—C10B—C5B	0.0	N4—C40—C41—C42	57.7 (2)
C6B—C5B—C10B—C9B	0.0	C46—C41—C42—C43	0.4 (3)
C4—C5B—C10B—C9B	−177.5 (8)	C40—C41—C42—C43	178.47 (18)
C3—N2—C11—C12	99.0 (2)	C41—C42—C43—C44	−0.4 (3)
C1—N2—C11—C12	−82.1 (2)	C42—C43—C44—C45	−0.1 (3)
N2—C11—C12—C13	−52.8 (3)	C43—C44—C45—C46	0.5 (3)
N2—C11—C12—C17	128.9 (2)	C42—C41—C46—C45	0.0 (3)
C17—C12—C13—C14	−0.7 (3)	C40—C41—C46—C45	−178.05 (18)
C11—C12—C13—C14	−179.06 (19)	C44—C45—C46—C41	−0.5 (3)
C12—C13—C14—C15	0.9 (3)	N3—C31—C47—C48	53.6 (2)
C13—C14—C15—C16	−0.5 (4)	C53—C31—C47—C48	−69.7 (2)
C14—C15—C16—C17	−0.1 (4)	C32—C31—C47—C48	167.01 (17)
C13—C12—C17—C16	0.1 (3)	N3—C31—C47—C52	−123.34 (18)
C11—C12—C17—C16	178.43 (19)	C53—C31—C47—C52	113.3 (2)
C15—C16—C17—C12	0.3 (3)	C32—C31—C47—C52	−9.9 (2)
N1—C2—C18—C19	169.36 (18)	C52—C47—C48—C49	2.6 (3)
C3—C2—C18—C19	−76.3 (2)	C31—C47—C48—C49	−174.44 (19)
C24—C2—C18—C19	47.7 (2)	C47—C48—C49—C50	−1.2 (4)
N1—C2—C18—C23	−12.6 (3)	C48—C49—C50—C51	−0.8 (4)
C3—C2—C18—C23	101.7 (2)	C49—C50—C51—C52	1.5 (4)
C24—C2—C18—C23	−134.4 (2)	C50—C51—C52—C47	−0.1 (3)
C23—C18—C19—C20	1.1 (3)	C48—C47—C52—C51	−2.0 (3)
C2—C18—C19—C20	179.1 (2)	C31—C47—C52—C51	174.91 (18)
C18—C19—C20—C21	−0.2 (4)	N3—C31—C53—C58	−161.27 (18)
C19—C20—C21—C22	−0.5 (4)	C47—C31—C53—C58	−40.9 (2)
C20—C21—C22—C23	0.1 (4)	C32—C31—C53—C58	83.8 (2)
C19—C18—C23—C22	−1.4 (3)	N3—C31—C53—C54	22.4 (2)
C2—C18—C23—C22	−179.4 (2)	C47—C31—C53—C54	142.79 (18)
C21—C22—C23—C18	0.8 (4)	C32—C31—C53—C54	−92.5 (2)
N1—C2—C24—C25	143.97 (18)	C58—C53—C54—C55	0.6 (3)
C18—C2—C24—C25	−92.7 (2)	C31—C53—C54—C55	177.0 (2)
C3—C2—C24—C25	29.5 (3)	C53—C54—C55—C56	−0.5 (4)
N1—C2—C24—C29	−36.5 (2)	C54—C55—C56—C57	0.0 (4)
C18—C2—C24—C29	86.8 (2)	C55—C56—C57—C58	0.4 (4)
C3—C2—C24—C29	−150.99 (19)	C56—C57—C58—C53	−0.3 (4)
C29—C24—C25—C26	0.3 (3)	C54—C53—C58—C57	−0.2 (3)
C2—C24—C25—C26	179.80 (19)	C31—C53—C58—C57	−176.6 (2)
C24—C25—C26—C27	0.5 (4)		

Hydrogen-bond geometry (Å, º)

Cg2, Cg3, Cg5, Cg8 and Cg9 are the centroids of the C5*A*–C10*A*, C12–C17, C24–C29, C41–C46 and C47–C52 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···S2^{i}	0.97	2.95	3.591 (2)	125
C4—H4*B*···*Cg*8^{ii}	0.97	2.97	3.693 (2)	133
C11—H11*B*···*Cg*9^{i}	0.97	2.83	3.524 (2)	129
C22—H22···*Cg*8^{iii}	0.93	2.77	3.554 (3)	143
C35—H35···*Cg*5	0.93	2.77	3.697 (3)	172
C40—H40*A*···*Cg*3^{ii}	0.97	2.81	3.556 (2)	134
C55—H55···*Cg*2^{iv}	0.93	2.84	3.725 (3)	160

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