Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structures of two new carbazole derivatives: ethyl 9-(benzenesulfonyl)-2-(4-fluoro-2-nitrophenyl)-6-methoxy-9*H*-carbazole-3-carboxylate and 12-(benzenesulfonyl)-12*H*-quinolino[4,3-*b*]carbazole

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Received 28 September 2022
Accepted 7 November 2022

Edited by S. Parkin, University of Kentucky, USA

Keywords: crystal structure; 9*H*-carbozole; quinoline; 9-(benzenesulfonyl); 2-nitrophenyl; 12-(benzenesulfonyl); 12*H*-indolo; phenanthridine; hydrogen bonding; Hirshfeld-surface analysis.

CCDC references: 2217905; 2217904

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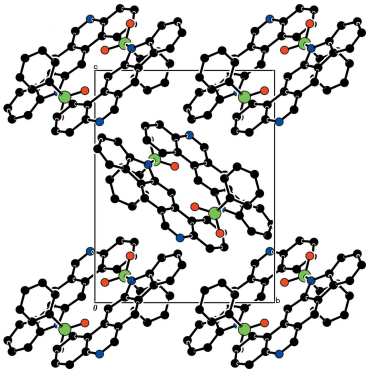
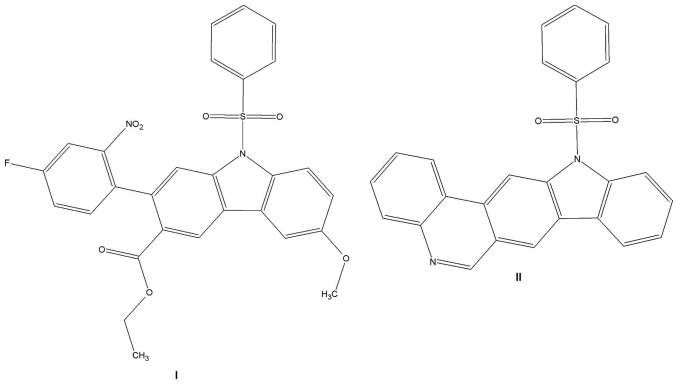
The title compounds, $C_{28}H_{21}FN_2O_7S$ (**I**) and $C_{25}H_{16}N_2O_2S$ (**II**), are carbazole derivatives with a benzenesulfonyl group attached to the carbazole moiety at the N atom on both molecules. A fluoro-substituted nitrophenyl ring system in **I** and a fused isoquinoline ring in **II** are attached to the respective carbazole moieties. In both compounds, the carbazole ring systems are essentially planar, with maximum deviations of 0.028 (2) and 0.026 (2) Å for carbon atoms in compounds **I** and **II**, respectively. The carbazole ring system is almost orthogonal to the benzene ring attached to sulfonyl group, with dihedral angles of 79.7 (2) in **I** and 88.2 (2)° in **II**, respectively. The mean planes of the carbazole ring systems make dihedral angles of 66.1 (2) and 1.3 (2)°, respectively, with the nitrophenyl ring in **I** and the planar isoquinoline moiety [maximum deviation of 0.009 (3) Å for a carbon atom in **II**, indicating that the ring system in **II** is essentially planar]. The benzenesulfonyl ring is almost normal to the isoquinoline ring, with a dihedral angle of 87.9 (2)° in **II** and the nitrophenyl ring forms a dihedral angle of 17.8 (2)° in **I**. In both compounds, intramolecular C—H···O hydrogen bonds generate *S*(6) ring motifs with the sulfone group O atoms. In crystals of compound **I**, the molecules are linked by C—H···O intermolecular weak hydrogen bonds, which generate *C*(7) and *C*(10) chains running parallel to [010] and [100], respectively.

1. Chemical context

Carbazole and its derivatives have been attractive to researchers because of their broad spectrum of biological activities. Beneficial properties include anti-oxidative (Tachibana *et al.*, 2001), antitumor activity against leukaemia, renal tumour, colon cancer and malignant melanoma tumour cell lines (Pindur & Lemster, 1997; Itoigawa *et al.*, 2000), anti-inflammatory and antimutagenic (Ramsewak *et al.*, 1999), antibiotic, antifungal and cytotoxic (Chakraborty *et al.*, 1965; 1978), pim kinase inhibitory (Giraud *et al.*, 2014), antimicrobial (Gu *et al.*, 2014), antimitotic and antioxidative activities (Tachibana *et al.*, 2003; Hu *et al.*, 2006), and anti-Alzheimer's effects (Thiratmatrakul *et al.*, 2014). Carbazole derivatives also exhibit electroactivity and luminescence, and are considered to be potential contenders for electronic applications such as luminescent and hole-transporting materials (Dijken *et al.*, 2004), colour displays (Santhanam & Sundaresan, 1986), organic semiconductors, high-performance



blue phosphorescent organic light-emitting diodes (Ye *et al.*, 2010), laser and solar cells (Friend, *et al.* 1999; Zhang *et al.* 2004). Carbazole-based heterocyclic polymer systems can be chemically or electrochemically polymerized to give products with a number of applications, such as rechargeable batteries (Sacak, 1999) and molecular glasses, which are widely studied as components of electroactive and photoactive materials (Zhang *et al.*, 2004). Against this background, the X-ray structure determinations of the title compounds, **I** and **II**, have been carried out and the results are presented here.



2. Structural commentary

In the molecular structures of the title compounds, $C_{28}H_{21}FN_2O_7S$ (**I**), which comprises a carbazole ring system attached to a benzenesulfonyl ring, a fluorine substituted nitrophenyl ring, a methoxy group and an ethylformate group and $C_{25}H_{16}N_2O_2S$ (**II**), which comprises a carbazole ring system attached to a benzenesulfonyl ring and fused isoquinoline ring, are illustrated in Figs. 1 and 2, respectively. In both compounds, the carbazole ring systems (N1/C1–C12) are essentially planar, with maximum deviations of 0.028 (2) and 0.026 (2) Å for atom C12 and C4 in compounds **I** and **II**, respectively. The carbazole ring system is almost orthogonal to the benzene ring (C20–C25) attached to the sulfonyl group, with dihedral angles of 79.7 (2) in **I** and 88.2 (2)° in **II**, respectively. The mean planes of the carbazole ring systems make dihedral angles of 66.1 (2) and 1.3 (2)°, respectively, with the nitrophenyl ring (C13–C18) in **I** and the planar isoquinoline (N2/C9/C10/C13–C19) moiety [maximum deviation of 0.009 (3) Å for atom C9] in **II**, indicating that the ring system in **II** is essentially planar. The benzenesulfonyl ring (C20–C25) is almost normal to the isoquinoline ring (N2/C9/C10/C13–C19), with a dihedral angle of 87.9 (2)° in **II**. In **I**, the corresponding dihedral angle with the nitrophenyl ring (C13–C18) is 17.8 (2)°.

In both compounds, the tetrahedral configuration is distorted around sulfur atom S1. The increase in the O2—S1—O1 angle [119.9 (2)° in **I** and 120.3 (2)° in **II**], with a simultaneous decrease in the N1—S1—C20 angle [104.7 (2)° in **I** and 104.9 (2)° in **II**] from the ideal tetrahedral value (109.5°) are attributed to the Thorpe-Ingold effect (Bassindale, 1984). The widening of the angles may be due to the repulsive interaction between the two short S=O bonds. The N1—C1 distances [1.434 (3) Å in **I** and 1.435 (3) Å in **II**] and N1—C12 bond lengths [1.421 (3) Å in **I** and 1.426 (3) Å in **II**] in the molecules are longer than the mean Nsp^2—Csp^2 bond-length value of 1.355 (14) Å (Allen *et al.*, 1987). The elongation observed may be due to the electron-withdrawing character of the benzenesulfonyl group. The sum of the bond angles around N1 (351.7° in **I** and 356.2° in **II**) indicate sp^2 hybridization. The geometric parameters of both compounds agree well with those of related structures (Narayanan *et al.*, 2014*a*,*b*).

In compound **I**, the nitro group is (+) syn-periplanar to the benzene ring (atoms C13–C18), as indicated by the values of the torsion angles C13—C14—N2—O6 = −24.6 (4)° and C15—C14—N2—O7 = −24.1 (4)°. The nitrogen atom N2 is almost in the plane of the benzene ring, with a torsion angle C18—C13—C14—N2 of −177.8 (2)°. The fluorine atom forms a torsion angle C14—C15—C16—F1 of 177.9 (2)°, indicating

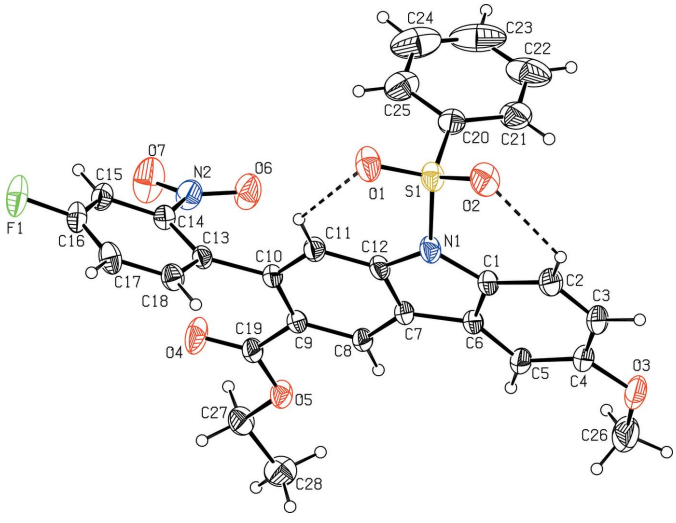


Figure 1
The molecular structure of compound **I**, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular contacts are shown as dashed lines (Table 1).

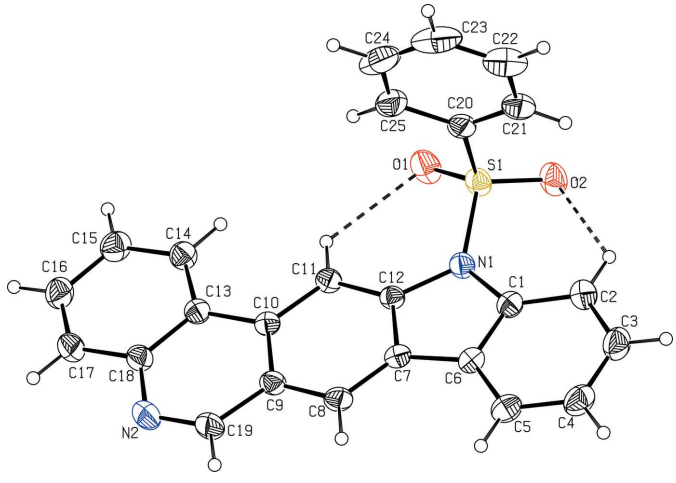


Figure 2
The molecular structure of compound **II**, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level. Intramolecular contacts are shown as dashed lines (Table 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2	0.93	2.36	2.945 (4)	121
C3—H3···O4^{i}	0.93	2.37	3.301 (3)	174
C11—H11···O1	0.93	2.35	2.952 (3)	123
C17—H17···O7^{ii}	0.93	2.50	3.428 (3)	173

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

that the fluorine substituent at C16 is almost coplanar with benzene ring C13–C18. The fluorine atom F1 deviates by −0.063 (2) Å from the benzene ring (C13–C18). In both compounds, the molecular structures are stabilized by C2—H2···O2 and C11—H11···O1 intramolecular interactions involving the sulfone oxygen atoms, which generate two $S(6)$ ring motifs (Fig. 1 and 2).

3. Supramolecular features

In the crystal packing of compound **I**, molecules are linked by C3—H3···O4^{i} and C17—H17···O7^{ii} (symmetry codes as per Table 1) intermolecular hydrogen bonds, generating $C(7)$ and $C(10)$ chains running parallel to [010] and [100], respectively. Very weak interactions between inversion-related C13–C18 and C20–C25 rings lead to an inter-centroid distance $Cg1\cdots Cg2^{iii}$ of 3.889 (2) Å [$Cg1$ and $Cg2$ are the centroids of rings C13–C18 and C20–C25, respectively, symmetry code: (iii) $1-x, 1-y, -z$]. No significant C—H···π interactions with centroid distances of less than ∼4 Å are observed in the structure.

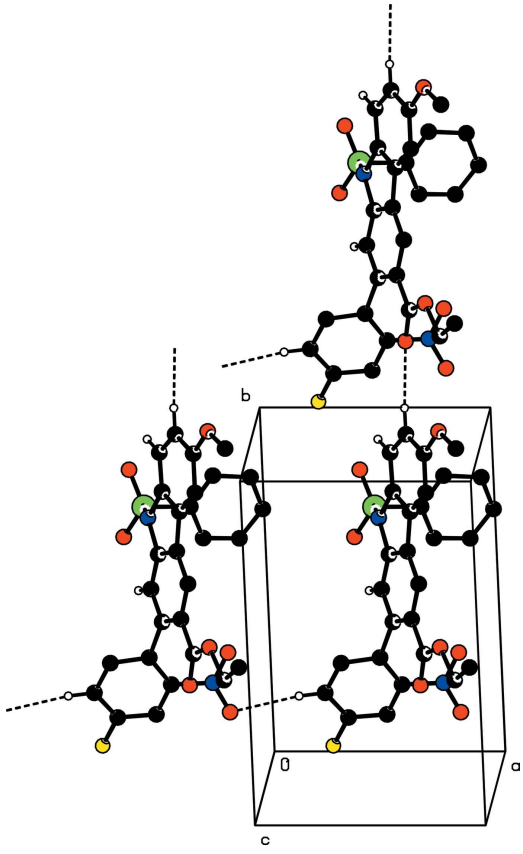


Figure 3
A view approximately down the a axis of the crystal packing of compound **I**. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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

$Cg1$ is the centroid of ring C13–C18 and $Cg2$ is the centroid of ring C7–C12.

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2	0.93	2.36	2.944 (4)	121
C11—H11···O1	0.93	2.34	2.940 (3)	122
C21—H21···N2^{i}	0.93	2.64	3.476 (4)	150
C4—H4···$Cg1^{ii}$	0.93	2.80	3.605 (4)	145
C16—H16···$Cg3^{iii}$	0.93	2.99	3.747 (3)	139

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

In compound **II**, the crystal packing is stabilized by C4—H4···$Cg1^{ii}$ and C16—H16···$Cg3^{iii}$ intermolecular interactions (symmetry codes as per Table 2), where $Cg1$ and $Cg3$ are the centres of gravity of rings (C13–C18) and (C7–C12), respectively. Packing plots of **I** and **II** are shown in Figs. 3 and 4. The whole of the fused ring system in **II** π-stacks with that of an inversion-related adjacent molecule, giving an interplanar spacing of 3.492 (3) Å.

4. Hirshfeld surface analysis

A recent article by Tiekink and collaborators (Tan *et al.*, 2019) reviews and describes the uses and utility of Hirshfeld-surface

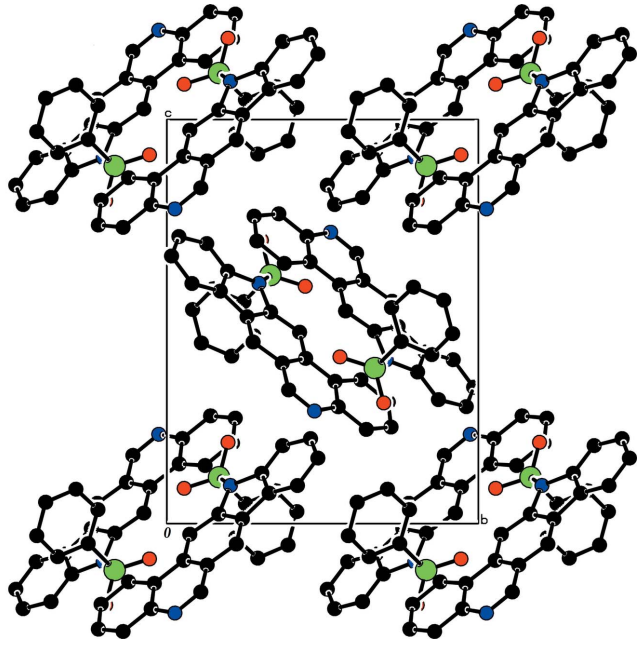


Figure 4
A view down the a axis of the crystal packing of compound **II**. Hydrogen bonds are shown as dashed lines.

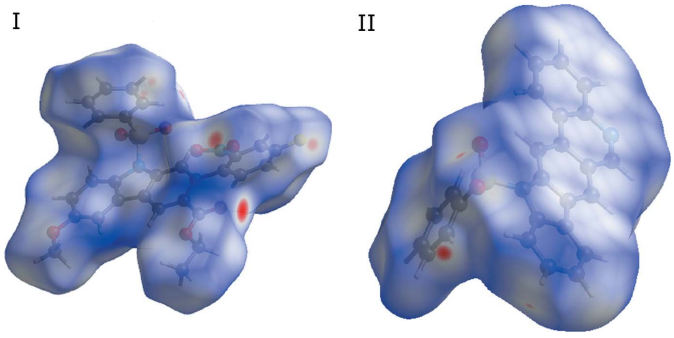


Figure 5
The Hirshfeld surfaces of compounds **I** and **II**, mapped over d_{norm}.

analysis (Spackman & Jayatilaka, 2009), and the associated two-dimensional fingerprint plots (McKinnon *et al.*, 2007), to analyse intermolecular contacts in crystals. The various analyses (d_{norm}, curvedness, shape index, and 2D-fingerprint plots) for **I** and **II** were performed with *CrystalExplorer17* (Turner *et al.*, 2017).

The Hirshfeld surfaces of compounds **I** and **II** mapped over d_{norm} are given in Fig. 5, and the intermolecular contacts are illustrated in Fig. 6*a* for **I** and Fig. 7*a* for **II**. They are colour-mapped with the normalized contact distance, d_{norm}, from red (distances shorter than the sum of the van der Waals radii) through white to blue (distances longer than the sum of the van der Waals radii), such that the red spots indicate intermolecular contacts involved in hydrogen bonding. The presence of interactions are indicated by red and blue areas on the shape-index surface (Fig. 6*b* for **I** and 7*b* for **II**). Areas on the Hirshfeld surface with high curvedness tend to divide the surface into contact patches with the neighbouring molecules. The coordination number in the crystal is thus indicated by the

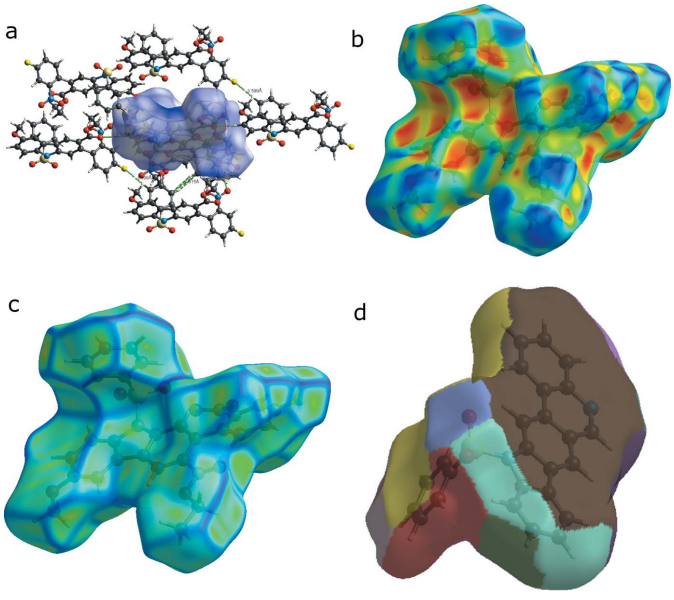


Figure 6
The Hirshfeld surfaces for visualizing the intermolecular contacts of compound **I**: (*a*) d_{norm}, showing the various intermolecular contacts in the crystal, (*b*) shape index, (*c*) curvedness and (*d*) fragment patches.

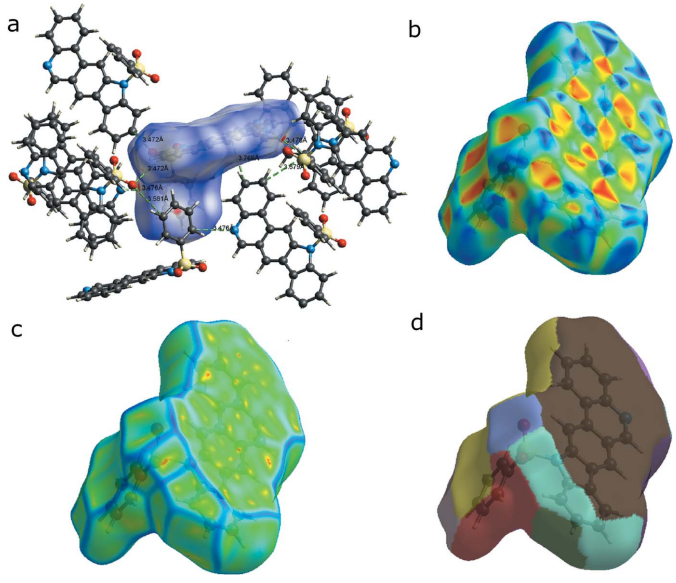


Figure 7
The Hirshfeld surfaces for visualizing the intermolecular contacts of compound **II**: (*a*) d_{norm}, showing the various intermolecular contacts in the crystal, (*b*) shape index, (*c*) curvedness and (*d*) fragment patches.

curvedness of the Hirshfeld surface (Fig. 6*c* for **I** and Fig. 7*c* for **II**). The nearest neighbour coordination environment of a molecule is indicated by colour patches on the Hirshfeld surface depending on their closeness to adjacent molecules (Fig. 6*d* for **I** and Fig. 7*d* for **II**).

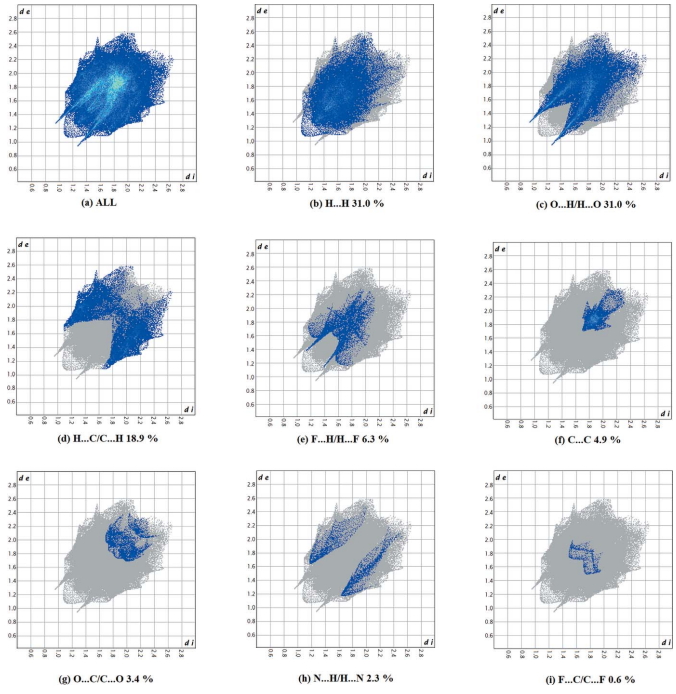


Figure 8
The full two-dimensional fingerprint plot for compound **I** (*a*) and plots delineated into (*b*) H···H, (*c*) O···H/H···O, (*d*) C···H/H···C, (*e*) F···H/H···F, (*f*) C···C, (*g*) O···C/C···O, (*h*) N···H/H···N, and (*i*) F···C/C···F contacts.

Table 3
Experimental details.

	I	II
Crystal data		
Chemical formula	$C_{28}H_{21}FN_2O_7S$	$C_{25}H_{16}N_2O_2S$
M_r	548.53	408.46
Crystal system, space group	Triclinic, $P\overline{1}$	Monoclinic, $P2_1/n$
Temperature (K)	298	296
a, b, c (Å)	8.1589 (9), 12.2053 (13), 12.9129 (13)	10.142 (1), 12.097 (1), 16.2218 (15)
α, β, γ (°)	101.569 (4), 93.086 (4), 92.481 (4)	90, 104.846 (4), 90
V (Å^3)	1256.0 (2)	1923.8 (3)
Z	2	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	0.19	0.19
Crystal size (mm)	0.31 × 0.24 × 0.13	0.40 × 0.35 × 0.25
Data collection		
Diffractometer	Bruker D8 Venture diffractometer with Photon II detector	Bruker D8 Venture diffractometer with Photon II detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.923, 0.965	0.867, 0.957
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	31739, 5194, 4176	60289, 4185, 3488
R_{int}	0.051	0.051
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.628	0.639
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.150, 1.13	0.054, 0.161, 1.13
No. of reflections	5194	4185
No. of parameters	354	271
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.38	0.32, −0.44

Computer programs: *APEX3*, *SAINT* and *XPREP* (Bruker, 2016), *SHELXT2018/2* (Sheldrick, 2008), *SHELXL2018/3* (Sheldrick, 2015), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2020).

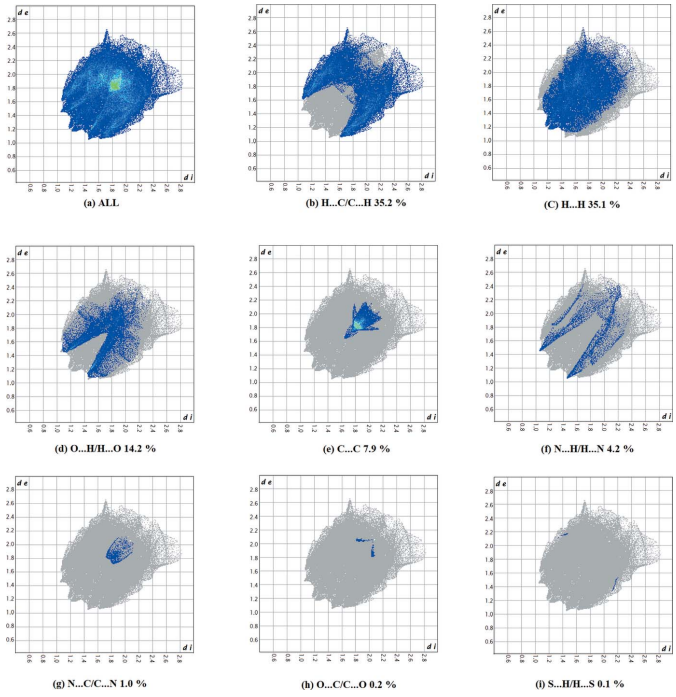


Figure 9
The full two-dimensional fingerprint plot for compound **II** (*a*) and plots delineated into (*b*) H···C/C···H, (*c*) H···H, (*d*) O···H/H···O, (*e*) C···C, (*f*) N···H/H···N, (*g*) N···C/C···N, (*h*) O···C/C···O and (*i*) S···H/H···S contacts.

Atom-contact fingerprint plots are given in Figs. 8 and 9. For compound **I**, they reveal the fraction of intermolecular contacts to be H···H = 31.0%, O···H/H···O = 31.0%, C···H/H···C = 18.9%, F···H/H···F = 6.3%, C···C = 4.9%, C···O/O···C = 3.4%, N···H/H···N = 2.3%, and C···F/F···C = 0.6%). For compound **II**, they reveal a similar trend, with the fraction of intermolecular contacts being C···H/H···C = 35.2%, H···H = 35.1%, O···H/H···O = 14.2%, C···C = 7.9%, N···H/H···N contacts = 4.2%, C···N/N···C contacts = 1.0%, C···O/O···C = 0.2% and S···H/H···S = 0.1%.

5. Synthesis and crystallization

Compound **I**: To a solution of ethyl (*E*)-3-{2-[(*E*)-4-fluoro-2-nitrostyryl]-5-methoxy-1-(benzenesulfonyl)-1*H*-indol-3-yl}-acrylate (3.0 g) in xylenes (100 mL), MnO_2 (2.5 g) was added, and the reaction mixture was refluxed for 12 h. It was then filtered through a celite pad and washed with hot xylenes (2 × 10 mL). The combined filtrate was concentrated under vacuum and then triturated with MeOH to give compound **I** (2.46 g, 85%) as a pale-yellow solid, mp: 473–475% K. Crystals of **I** were obtained by re-crystallization from ethanol.

Compound **II**: To a solution of 2-(2-nitrophenyl)-9-(benzenesulfonyl)-9*H*-carbazole-3-carbaldehyde (1.0 g) in dry THF (50 mL), Raney-Ni (2.0 g) was carefully added, and the reaction mixture was stirred at room temperature for 3 h. Then, the nickel residue was carefully filtered through a celite

pad and washed with hot THF (3 × 30 mL). The combined filtrate was evaporated under vacuum and then triturated with MeOH to give compound **II** (0.79 g, 80%) as a white solid, mp: 487–489 K. Crystals suitable for X-ray analysis were obtained by re-crystallization from ethanol.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The positions of hydrogen atoms were found in difference electron-density maps. Hydrogen atoms bound to carbon were treated as riding atoms, with d(C—H) = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C) (methyl). Methyl group torsion angles were optimized.

Acknowledgements

The authors thank the SAIF, IIT, Madras, India, for the data collection.

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supporting information

Acta Cryst. (2022). E**78**, 1198-1203 [https://doi.org/10.1107/S2056989022010684]

Crystal structures of two new carbazole derivatives: ethyl 9-(benzenesulfonyl)-2-(4-fluoro-2-nitrophenyl)-6-methoxy-9*H*-carbazole-3-carboxylate and 12-(benzenesulfonyl)-12*H*-quinolino[4,3-*b*]carbazole

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Computing details

For both structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *APEX3*/*SAINT* (Bruker, 2016); data reduction: *SAINT*/*XPREP* (Bruker, 2016); program(s) used to solve structure: *SHELXT2018/2* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2020).

Ethyl 9-(benzenesulfonyl)-2-(4-fluoro-2-nitrophenyl)-6-methoxy-9*H*-carbazole-3-carboxylate (I)

Crystal data

$C_{28}H_{21}FN_2O_7S$
M_r = 548.53
Triclinic, $P\overline{1}$
a = 8.1589 (9) Å
b = 12.2053 (13) Å
c = 12.9129 (13) Å
α = 101.569 (4)°
β = 93.086 (4)°
γ = 92.481 (4)°
V = 1256.0 (2) Å^3
Z = 2
$F(000)$ = 568
D_x = 1.450 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9133 reflections
θ = 2.9–20.6°
μ = 0.19 mm^{-1}
T = 298 K
Solid, pale yellow
0.31 × 0.24 × 0.13 mm

Data collection

Bruker D8 Venture diffractometer with Photon II detector
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.923, T_{max} = 0.965
31739 measured reflections
5194 independent reflections
4176 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 26.5°, θ_{min} = 3.2°
h = −10→10
k = −15→15
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.150
S = 1.13
5194 reflections

354 parameters	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.9577P]$
0 restraints	where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.28$ e Å^{-3}
	$\Delta\rho_{min} = -0.38$ e Å^{-3}

Special details

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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.5947 (3)	0.82807 (19)	0.33841 (19)	0.0432 (5)
C2	0.5905 (4)	0.9424 (2)	0.3415 (2)	0.0547 (7)
H2	0.534951	0.969581	0.287941	0.066*
C3	0.6708 (4)	1.0137 (2)	0.4262 (2)	0.0602 (8)
H3	0.670280	1.090490	0.429413	0.072*
C4	0.7534 (4)	0.9746 (2)	0.5077 (2)	0.0550 (7)
C5	0.7536 (3)	0.8609 (2)	0.5069 (2)	0.0484 (6)
H5	0.805234	0.834352	0.562212	0.058*
C6	0.6741 (3)	0.78757 (18)	0.42037 (19)	0.0413 (5)
C7	0.6522 (3)	0.66650 (18)	0.39461 (18)	0.0384 (5)
C8	0.7000 (3)	0.58302 (18)	0.44653 (18)	0.0382 (5)
H8	0.760023	0.601797	0.511504	0.046*
C9	0.6584 (3)	0.47101 (18)	0.40159 (18)	0.0369 (5)
C10	0.5673 (3)	0.44179 (18)	0.30303 (18)	0.0369 (5)
C11	0.5192 (3)	0.52566 (19)	0.25104 (19)	0.0411 (5)
H11	0.458835	0.507465	0.186175	0.049*
C12	0.5621 (3)	0.63664 (18)	0.29683 (19)	0.0390 (5)
C13	0.4990 (3)	0.32669 (18)	0.25064 (17)	0.0359 (5)
C14	0.5846 (3)	0.23731 (19)	0.19937 (19)	0.0397 (5)
C15	0.5085 (3)	0.1383 (2)	0.1430 (2)	0.0461 (6)
H15	0.569368	0.080494	0.109286	0.055*
C16	0.3402 (3)	0.1284 (2)	0.1385 (2)	0.0479 (6)
C17	0.2487 (3)	0.2110 (2)	0.1896 (2)	0.0508 (6)
H17	0.134812	0.201332	0.187587	0.061*
C18	0.3288 (3)	0.3093 (2)	0.2444 (2)	0.0441 (5)
H18	0.266421	0.366080	0.278478	0.053*
C19	0.7117 (3)	0.38165 (19)	0.45764 (19)	0.0422 (5)
C20	0.6890 (3)	0.7300 (2)	0.0857 (2)	0.0506 (6)
C21	0.7943 (4)	0.8241 (3)	0.1038 (2)	0.0722 (9)
H21	0.761507	0.893146	0.138596	0.087*
C22	0.9537 (6)	0.8117 (5)	0.0674 (3)	0.1089 (18)
H22	1.029701	0.872575	0.079031	0.131*
C23	0.9955 (6)	0.7078 (7)	0.0144 (3)	0.120 (2)
H23	1.101471	0.699221	−0.008005	0.143*

C24	0.8868 (7)	0.6181 (5)	−0.0060 (3)	0.1110 (17)
H24	0.916615	0.550314	−0.045527	0.133*
C25	0.7336 (5)	0.6269 (3)	0.0313 (3)	0.0739 (9)
H25	0.660166	0.564583	0.020359	0.089*
C26	0.9088 (6)	1.0250 (3)	0.6723 (3)	0.0956 (14)
H26A	0.830154	0.991505	0.711004	0.143*
H26B	0.962806	1.089934	0.717734	0.143*
H26C	0.988796	0.971938	0.647947	0.143*
C27	0.8536 (4)	0.3375 (2)	0.6062 (2)	0.0535 (7)
H27A	0.934315	0.294924	0.565185	0.064*
H27B	0.764671	0.286048	0.616283	0.064*
C28	0.9307 (4)	0.3968 (3)	0.7108 (2)	0.0673 (8)
H28A	1.013542	0.451088	0.700178	0.101*
H28B	0.980023	0.343642	0.746679	0.101*
H28C	0.848189	0.434050	0.752872	0.101*
N1	0.5207 (3)	0.73549 (16)	0.26146 (17)	0.0445 (5)
N2	0.7653 (3)	0.2432 (2)	0.2032 (2)	0.0580 (6)
O1	0.3949 (3)	0.64184 (17)	0.08549 (17)	0.0671 (6)
O2	0.4347 (3)	0.84684 (17)	0.12977 (17)	0.0676 (6)
O3	0.8282 (3)	1.05644 (16)	0.58552 (18)	0.0792 (7)
O4	0.6862 (3)	0.28366 (15)	0.42290 (17)	0.0798 (8)
O5	0.7909 (2)	0.42120 (13)	0.55099 (14)	0.0494 (4)
O6	0.8380 (3)	0.33442 (19)	0.2187 (2)	0.0800 (7)
O7	0.8334 (3)	0.1550 (2)	0.1902 (3)	0.0957 (9)
S1	0.49241 (8)	0.73975 (5)	0.13348 (5)	0.0483 (2)
F1	0.2637 (2)	0.03387 (13)	0.08098 (16)	0.0748 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0559 (15)	0.0285 (11)	0.0468 (13)	0.0031 (10)	0.0074 (11)	0.0106 (10)
C2	0.0776 (19)	0.0340 (13)	0.0562 (16)	0.0105 (12)	0.0076 (14)	0.0156 (11)
C3	0.093 (2)	0.0257 (12)	0.0631 (17)	0.0059 (13)	0.0135 (16)	0.0100 (11)
C4	0.079 (2)	0.0314 (13)	0.0523 (15)	−0.0046 (12)	0.0100 (14)	0.0029 (11)
C5	0.0657 (17)	0.0318 (12)	0.0465 (14)	−0.0009 (11)	0.0030 (12)	0.0058 (10)
C6	0.0529 (14)	0.0288 (11)	0.0435 (13)	0.0018 (10)	0.0076 (10)	0.0096 (9)
C7	0.0481 (13)	0.0276 (11)	0.0405 (12)	0.0004 (9)	0.0048 (10)	0.0092 (9)
C8	0.0482 (13)	0.0292 (11)	0.0376 (11)	0.0007 (9)	0.0017 (10)	0.0086 (9)
C9	0.0443 (12)	0.0296 (11)	0.0385 (12)	0.0012 (9)	0.0044 (9)	0.0104 (9)
C10	0.0420 (12)	0.0292 (11)	0.0401 (12)	−0.0001 (9)	0.0052 (9)	0.0081 (9)
C11	0.0480 (13)	0.0348 (12)	0.0404 (12)	−0.0019 (10)	−0.0029 (10)	0.0099 (9)
C12	0.0456 (13)	0.0305 (11)	0.0439 (12)	0.0007 (9)	0.0023 (10)	0.0154 (9)
C13	0.0411 (12)	0.0292 (11)	0.0385 (11)	−0.0011 (9)	0.0011 (9)	0.0107 (9)
C14	0.0394 (12)	0.0350 (12)	0.0443 (12)	−0.0005 (9)	0.0022 (10)	0.0078 (9)
C15	0.0554 (15)	0.0312 (12)	0.0497 (14)	0.0025 (10)	−0.0027 (11)	0.0048 (10)
C16	0.0517 (15)	0.0316 (12)	0.0585 (15)	−0.0067 (10)	−0.0146 (12)	0.0110 (11)
C17	0.0379 (13)	0.0437 (14)	0.0729 (18)	−0.0046 (11)	−0.0077 (12)	0.0214 (13)
C18	0.0414 (13)	0.0374 (12)	0.0554 (14)	0.0046 (10)	0.0038 (11)	0.0135 (11)

C19	0.0546 (14)	0.0307 (12)	0.0427 (13)	0.0006 (10)	0.0019 (11)	0.0113 (9)
C20	0.0607 (16)	0.0537 (15)	0.0379 (13)	0.0025 (12)	−0.0091 (11)	0.0141 (11)
C21	0.074 (2)	0.091 (2)	0.0472 (16)	−0.0215 (18)	−0.0042 (15)	0.0091 (16)
C22	0.081 (3)	0.191 (5)	0.052 (2)	−0.043 (3)	−0.0110 (19)	0.033 (3)
C23	0.078 (3)	0.235 (7)	0.050 (2)	0.042 (4)	−0.001 (2)	0.035 (3)
C24	0.122 (4)	0.153 (5)	0.064 (2)	0.075 (4)	0.005 (3)	0.023 (3)
C25	0.098 (3)	0.071 (2)	0.0551 (18)	0.0295 (19)	−0.0012 (17)	0.0137 (15)
C26	0.144 (4)	0.065 (2)	0.068 (2)	−0.032 (2)	−0.022 (2)	0.0060 (18)
C27	0.0665 (17)	0.0436 (14)	0.0554 (16)	0.0101 (12)	−0.0020 (13)	0.0220 (12)
C28	0.076 (2)	0.072 (2)	0.0559 (17)	0.0126 (16)	−0.0095 (15)	0.0197 (15)
N1	0.0546 (12)	0.0305 (10)	0.0508 (12)	0.0017 (9)	−0.0021 (9)	0.0155 (9)
N2	0.0448 (13)	0.0518 (14)	0.0717 (16)	−0.0017 (11)	0.0119 (11)	−0.0023 (11)
O1	0.0753 (14)	0.0557 (12)	0.0692 (13)	−0.0174 (10)	−0.0300 (11)	0.0238 (10)
O2	0.0830 (15)	0.0528 (12)	0.0743 (14)	0.0187 (10)	−0.0081 (11)	0.0302 (10)
O3	0.128 (2)	0.0355 (10)	0.0670 (14)	−0.0149 (11)	−0.0070 (13)	0.0004 (9)
O4	0.142 (2)	0.0282 (10)	0.0659 (13)	−0.0011 (11)	−0.0335 (13)	0.0130 (9)
O5	0.0695 (12)	0.0319 (8)	0.0475 (10)	0.0026 (8)	−0.0100 (8)	0.0134 (7)
O6	0.0534 (12)	0.0631 (14)	0.1118 (19)	−0.0173 (11)	0.0258 (12)	−0.0109 (13)
O7	0.0493 (13)	0.0665 (15)	0.163 (3)	0.0153 (11)	0.0119 (15)	−0.0009 (16)
S1	0.0555 (4)	0.0389 (3)	0.0527 (4)	0.0009 (3)	−0.0122 (3)	0.0189 (3)
F1	0.0759 (12)	0.0370 (8)	0.1018 (14)	−0.0127 (8)	−0.0333 (10)	0.0047 (8)

Geometric parameters (Å, º)

C1—C2	1.390 (3)	C17—H17	0.9300
C1—C6	1.396 (3)	C18—H18	0.9300
C1—N1	1.434 (3)	C19—O4	1.195 (3)
C2—C3	1.369 (4)	C19—O5	1.326 (3)
C2—H2	0.9300	C20—C21	1.377 (4)
C3—C4	1.395 (4)	C20—C25	1.387 (4)
C3—H3	0.9300	C20—S1	1.749 (3)
C4—O3	1.363 (3)	C21—C22	1.411 (6)
C4—C5	1.386 (3)	C21—H21	0.9300
C5—C6	1.393 (3)	C22—C23	1.381 (8)
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.449 (3)	C23—C24	1.352 (7)
C7—C8	1.386 (3)	C23—H23	0.9300
C7—C12	1.400 (3)	C24—C25	1.365 (6)
C8—C9	1.393 (3)	C24—H24	0.9300
C8—H8	0.9300	C25—H25	0.9300
C9—C10	1.412 (3)	C26—O3	1.397 (4)
C9—C19	1.492 (3)	C26—H26A	0.9600
C10—C11	1.391 (3)	C26—H26B	0.9600
C10—C13	1.501 (3)	C26—H26C	0.9600
C11—C12	1.387 (3)	C27—O5	1.454 (3)
C11—H11	0.9300	C27—C28	1.490 (4)
C12—N1	1.421 (3)	C27—H27A	0.9700
C13—C18	1.392 (3)	C27—H27B	0.9700

C13—C14	1.393 (3)	C28—H28A	0.9600
C14—C15	1.381 (3)	C28—H28B	0.9600
C14—N2	1.471 (3)	C28—H28C	0.9600
C15—C16	1.371 (4)	N1—S1	1.668 (2)
C15—H15	0.9300	N2—O6	1.213 (3)
C16—F1	1.348 (3)	N2—O7	1.219 (3)
C16—C17	1.363 (4)	O1—S1	1.419 (2)
C17—C18	1.382 (3)	O2—S1	1.4172 (19)
C2—C1—C6	121.1 (2)	O4—C19—O5	122.6 (2)
C2—C1—N1	129.8 (2)	O4—C19—C9	124.0 (2)
C6—C1—N1	109.12 (19)	O5—C19—C9	113.48 (19)
C3—C2—C1	117.7 (3)	C21—C20—C25	122.3 (3)
C3—C2—H2	121.1	C21—C20—S1	119.3 (2)
C1—C2—H2	121.1	C25—C20—S1	118.5 (3)
C2—C3—C4	121.9 (2)	C20—C21—C22	117.5 (4)
C2—C3—H3	119.0	C20—C21—H21	121.3
C4—C3—H3	119.0	C22—C21—H21	121.3
O3—C4—C5	124.8 (3)	C23—C22—C21	119.1 (4)
O3—C4—C3	114.5 (2)	C23—C22—H22	120.5
C5—C4—C3	120.7 (3)	C21—C22—H22	120.5
C4—C5—C6	117.8 (2)	C24—C23—C22	122.0 (5)
C4—C5—H5	121.1	C24—C23—H23	119.0
C6—C5—H5	121.1	C22—C23—H23	119.0
C5—C6—C1	120.8 (2)	C23—C24—C25	120.1 (5)
C5—C6—C7	131.9 (2)	C23—C24—H24	119.9
C1—C6—C7	107.3 (2)	C25—C24—H24	119.9
C8—C7—C12	119.1 (2)	C24—C25—C20	119.0 (4)
C8—C7—C6	133.2 (2)	C24—C25—H25	120.5
C12—C7—C6	107.7 (2)	C20—C25—H25	120.5
C7—C8—C9	120.1 (2)	O3—C26—H26A	109.5
C7—C8—H8	119.9	O3—C26—H26B	109.5
C9—C8—H8	119.9	H26A—C26—H26B	109.5
C8—C9—C10	120.3 (2)	O3—C26—H26C	109.5
C8—C9—C19	119.7 (2)	H26A—C26—H26C	109.5
C10—C9—C19	120.0 (2)	H26B—C26—H26C	109.5
C11—C10—C9	119.5 (2)	O5—C27—C28	108.0 (2)
C11—C10—C13	114.0 (2)	O5—C27—H27A	110.1
C9—C10—C13	126.16 (19)	C28—C27—H27A	110.1
C12—C11—C10	119.4 (2)	O5—C27—H27B	110.1
C12—C11—H11	120.3	C28—C27—H27B	110.1
C10—C11—H11	120.3	H27A—C27—H27B	108.4
C11—C12—C7	121.5 (2)	C27—C28—H28A	109.5
C11—C12—N1	129.3 (2)	C27—C28—H28B	109.5
C7—C12—N1	109.07 (19)	H28A—C28—H28B	109.5
C18—C13—C14	115.5 (2)	C27—C28—H28C	109.5
C18—C13—C10	116.5 (2)	H28A—C28—H28C	109.5
C14—C13—C10	127.7 (2)	H28B—C28—H28C	109.5

C15—C14—C13	123.4 (2)	C12—N1—C1	106.72 (19)
C15—C14—N2	115.6 (2)	C12—N1—S1	122.61 (17)
C13—C14—N2	121.0 (2)	C1—N1—S1	122.44 (16)
C16—C15—C14	117.6 (2)	O6—N2—O7	123.7 (2)
C16—C15—H15	121.2	O6—N2—C14	118.9 (2)
C14—C15—H15	121.2	O7—N2—C14	117.4 (2)
F1—C16—C17	119.4 (2)	C4—O3—C26	118.4 (2)
F1—C16—C15	118.4 (2)	C19—O5—C27	115.66 (19)
C17—C16—C15	122.1 (2)	O2—S1—O1	119.94 (13)
C16—C17—C18	118.6 (2)	O2—S1—N1	106.24 (12)
C16—C17—H17	120.7	O1—S1—N1	106.37 (11)
C18—C17—H17	120.7	O2—S1—C20	109.43 (14)
C17—C18—C13	122.6 (2)	O1—S1—C20	109.01 (14)
C17—C18—H18	118.7	N1—S1—C20	104.74 (11)
C13—C18—H18	118.7		

C6—C1—C2—C3	1.9 (4)	C15—C16—C17—C18	2.4 (4)
N1—C1—C2—C3	178.9 (3)	C16—C17—C18—C13	−0.9 (4)
C1—C2—C3—C4	−0.6 (5)	C14—C13—C18—C17	−1.1 (3)
C2—C3—C4—O3	179.4 (3)	C10—C13—C18—C17	173.7 (2)
C2—C3—C4—C5	−1.5 (5)	C8—C9—C19—O4	−177.3 (3)
O3—C4—C5—C6	−178.7 (3)	C10—C9—C19—O4	2.2 (4)
C3—C4—C5—C6	2.3 (4)	C8—C9—C19—O5	2.9 (3)
C4—C5—C6—C1	−1.0 (4)	C10—C9—C19—O5	−177.6 (2)
C4—C5—C6—C7	179.7 (3)	C25—C20—C21—C22	−1.9 (4)
C2—C1—C6—C5	−1.1 (4)	S1—C20—C21—C22	177.6 (2)
N1—C1—C6—C5	−178.7 (2)	C20—C21—C22—C23	1.2 (5)
C2—C1—C6—C7	178.4 (2)	C21—C22—C23—C24	1.6 (6)
N1—C1—C6—C7	0.8 (3)	C22—C23—C24—C25	−3.8 (7)
C5—C6—C7—C8	0.9 (5)	C23—C24—C25—C20	3.1 (6)
C1—C6—C7—C8	−178.5 (3)	C21—C20—C25—C24	−0.2 (5)
C5—C6—C7—C12	−179.8 (3)	S1—C20—C25—C24	−179.7 (3)
C1—C6—C7—C12	0.9 (3)	C11—C12—N1—C1	179.3 (2)
C12—C7—C8—C9	−0.1 (4)	C7—C12—N1—C1	2.6 (3)
C6—C7—C8—C9	179.2 (2)	C11—C12—N1—S1	−31.7 (4)
C7—C8—C9—C10	0.0 (3)	C7—C12—N1—S1	151.62 (18)
C7—C8—C9—C19	179.5 (2)	C2—C1—N1—C12	−179.4 (3)
C8—C9—C10—C11	0.0 (3)	C6—C1—N1—C12	−2.1 (3)
C19—C9—C10—C11	−179.5 (2)	C2—C1—N1—S1	31.5 (4)
C8—C9—C10—C13	−173.3 (2)	C6—C1—N1—S1	−151.14 (19)
C19—C9—C10—C13	7.2 (4)	C15—C14—N2—O6	155.8 (3)
C9—C10—C11—C12	0.2 (4)	C13—C14—N2—O6	−24.6 (4)
C13—C10—C11—C12	174.2 (2)	C15—C14—N2—O7	−24.1 (4)
C10—C11—C12—C7	−0.3 (4)	C13—C14—N2—O7	155.5 (3)
C10—C11—C12—N1	−176.7 (2)	C5—C4—O3—C26	−1.4 (5)
C8—C7—C12—C11	0.2 (4)	C3—C4—O3—C26	177.7 (3)
C6—C7—C12—C11	−179.2 (2)	O4—C19—O5—C27	3.4 (4)
C8—C7—C12—N1	177.3 (2)	C9—C19—O5—C27	−176.7 (2)

C6—C7—C12—N1	−2.2 (3)	C28—C27—O5—C19	−177.3 (2)
C11—C10—C13—C18	−62.6 (3)	C12—N1—S1—O2	173.3 (2)
C9—C10—C13—C18	110.9 (3)	C1—N1—S1—O2	−42.4 (2)
C11—C10—C13—C14	111.5 (3)	C12—N1—S1—O1	44.5 (2)
C9—C10—C13—C14	−75.0 (3)	C1—N1—S1—O1	−171.3 (2)
C18—C13—C14—C15	1.8 (3)	C12—N1—S1—C20	−70.9 (2)
C10—C13—C14—C15	−172.4 (2)	C1—N1—S1—C20	73.4 (2)
C18—C13—C14—N2	−177.8 (2)	C21—C20—S1—O2	33.8 (3)
C10—C13—C14—N2	8.1 (4)	C25—C20—S1—O2	−146.8 (2)
C13—C14—C15—C16	−0.4 (4)	C21—C20—S1—O1	166.7 (2)
N2—C14—C15—C16	179.1 (2)	C25—C20—S1—O1	−13.8 (2)
C14—C15—C16—F1	177.9 (2)	C21—C20—S1—N1	−79.8 (2)
C14—C15—C16—C17	−1.7 (4)	C25—C20—S1—N1	99.7 (2)
F1—C16—C17—C18	−177.2 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2	0.93	2.36	2.945 (4)	121
C3—H3···O4^{i}	0.93	2.37	3.301 (3)	174
C11—H11···O1	0.93	2.35	2.952 (3)	123
C17—H17···O7^{ii}	0.93	2.50	3.428 (3)	173

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

12-(Benzenesulfonyl)-12*H*-quinolino[4,3-*b*]carbazole (II)

Crystal data

$C_{25}H_{16}N_2O_2S$
M_r = 408.46
Monoclinic, $P2_1/n$
a = 10.142 (1) Å
b = 12.097 (1) Å
c = 16.2218 (15) Å
β = 104.846 (4)°
V = 1923.8 (3) Å^3
Z = 4
$F(000)$ = 848
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9986 reflections
θ = 2.7–29.5°
μ = 0.19 mm^{-1}
T = 296 K
Solid, colourless
0.40 × 0.35 × 0.25 mm

Data collection

Bruker D8 Venture
diffractometer with Photon II detector
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan
(SADABS; Bruker, 2016)
T_{min} = 0.867, T_{max} = 0.957
60289 measured reflections
4185 independent reflections
3488 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.0°, θ_{min} = 3.3°
h = −12→12
k = −15→15
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.161$
$S = 1.13$
4185 reflections
271 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 2.5552P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Special details

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8659 (3)	0.1951 (2)	0.62473 (17)	0.0405 (6)
C2	0.8576 (3)	0.1281 (3)	0.69302 (19)	0.0518 (7)
H2	0.796204	0.142990	0.725444	0.062*
C3	0.9447 (3)	0.0387 (3)	0.7104 (2)	0.0592 (8)
H3	0.941923	−0.007334	0.755800	0.071*
C4	1.0364 (3)	0.0151 (3)	0.6623 (2)	0.0576 (8)
H4	1.094393	−0.045445	0.676287	0.069*
C5	1.0418 (3)	0.0807 (2)	0.5943 (2)	0.0515 (7)
H5	1.102062	0.064446	0.561328	0.062*
C6	0.9560 (3)	0.1717 (2)	0.57542 (16)	0.0391 (5)
C7	0.9415 (2)	0.2576 (2)	0.51200 (16)	0.0368 (5)
C8	1.0084 (3)	0.2769 (2)	0.44958 (17)	0.0427 (6)
H8	1.075496	0.228451	0.441961	0.051*
C9	0.9744 (3)	0.3705 (2)	0.39769 (16)	0.0392 (6)
C10	0.8736 (2)	0.4456 (2)	0.40903 (15)	0.0340 (5)
C11	0.8069 (3)	0.4262 (2)	0.47373 (15)	0.0363 (5)
H11	0.741028	0.474851	0.482689	0.044*
C12	0.8418 (2)	0.3330 (2)	0.52353 (15)	0.0340 (5)
C13	0.8459 (2)	0.5400 (2)	0.35213 (15)	0.0372 (5)
C14	0.7505 (3)	0.6228 (2)	0.35608 (18)	0.0457 (6)
H14	0.701230	0.617974	0.397050	0.055*
C15	0.7285 (3)	0.7109 (3)	0.3006 (2)	0.0543 (7)
H15	0.664791	0.764658	0.304288	0.065*
C16	0.8013 (3)	0.7197 (3)	0.2390 (2)	0.0562 (8)
H16	0.786655	0.779570	0.201767	0.067*
C17	0.8941 (3)	0.6405 (3)	0.2332 (2)	0.0533 (7)
H17	0.941880	0.646462	0.191462	0.064*
C18	0.9187 (3)	0.5501 (2)	0.28923 (17)	0.0432 (6)
C19	1.0408 (3)	0.3910 (3)	0.33103 (19)	0.0523 (7)
H19	1.107016	0.340809	0.324773	0.063*

C20	0.5258 (3)	0.2476 (3)	0.54943 (17)	0.0464 (6)
C21	0.4892 (3)	0.1494 (3)	0.5817 (2)	0.0557 (8)
H21	0.529794	0.128664	0.637693	0.067*
C22	0.3916 (4)	0.0826 (3)	0.5298 (3)	0.0770 (11)
H22	0.364572	0.017708	0.551609	0.092*
C23	0.3347 (4)	0.1110 (5)	0.4470 (3)	0.0920 (16)
H23	0.270298	0.064956	0.412217	0.110*
C24	0.3727 (4)	0.2082 (5)	0.4147 (3)	0.0880 (15)
H24	0.333913	0.226625	0.358053	0.106*
C25	0.4677 (3)	0.2788 (4)	0.4653 (2)	0.0656 (9)
H25	0.491861	0.344837	0.443700	0.079*
N1	0.7952 (2)	0.29582 (18)	0.59462 (14)	0.0400 (5)
N2	1.0159 (3)	0.4741 (2)	0.27880 (17)	0.0562 (7)
O1	0.6239 (2)	0.44428 (18)	0.58737 (15)	0.0610 (6)
O2	0.6604 (2)	0.30363 (18)	0.70130 (12)	0.0553 (5)
S1	0.64894 (7)	0.33247 (6)	0.61490 (4)	0.0440 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0408 (13)	0.0378 (13)	0.0409 (13)	0.0012 (11)	0.0070 (11)	0.0004 (10)
C2	0.0532 (17)	0.0534 (17)	0.0502 (16)	0.0005 (14)	0.0156 (13)	0.0084 (13)
C3	0.0629 (19)	0.0517 (18)	0.0594 (18)	−0.0013 (15)	0.0089 (15)	0.0174 (15)
C4	0.0558 (18)	0.0442 (16)	0.067 (2)	0.0085 (14)	0.0056 (15)	0.0108 (14)
C5	0.0474 (16)	0.0465 (16)	0.0583 (17)	0.0119 (13)	0.0097 (13)	0.0023 (13)
C6	0.0380 (13)	0.0377 (13)	0.0392 (13)	0.0019 (10)	0.0056 (10)	−0.0006 (10)
C7	0.0323 (12)	0.0378 (13)	0.0386 (12)	0.0026 (10)	0.0061 (10)	−0.0032 (10)
C8	0.0375 (13)	0.0437 (14)	0.0492 (15)	0.0108 (11)	0.0156 (11)	−0.0018 (11)
C9	0.0358 (13)	0.0451 (14)	0.0386 (13)	0.0029 (11)	0.0131 (10)	−0.0029 (11)
C10	0.0328 (11)	0.0337 (12)	0.0344 (12)	−0.0022 (9)	0.0064 (9)	−0.0052 (9)
C11	0.0374 (12)	0.0339 (12)	0.0393 (13)	0.0030 (10)	0.0129 (10)	−0.0036 (10)
C12	0.0325 (11)	0.0363 (12)	0.0336 (11)	0.0011 (10)	0.0093 (9)	−0.0038 (9)
C13	0.0360 (12)	0.0379 (13)	0.0361 (12)	−0.0052 (10)	0.0061 (10)	−0.0041 (10)
C14	0.0477 (15)	0.0428 (14)	0.0475 (15)	0.0013 (12)	0.0138 (12)	0.0013 (12)
C15	0.0539 (17)	0.0420 (15)	0.0649 (19)	0.0036 (13)	0.0114 (14)	0.0058 (14)
C16	0.0565 (18)	0.0482 (17)	0.0610 (19)	−0.0062 (14)	0.0096 (14)	0.0149 (14)
C17	0.0498 (16)	0.0584 (18)	0.0536 (17)	−0.0098 (14)	0.0169 (13)	0.0094 (14)
C18	0.0402 (14)	0.0464 (15)	0.0437 (14)	−0.0050 (11)	0.0118 (11)	0.0009 (11)
C19	0.0480 (16)	0.0606 (18)	0.0554 (17)	0.0123 (14)	0.0263 (13)	0.0040 (14)
C20	0.0378 (13)	0.0620 (18)	0.0432 (14)	0.0135 (12)	0.0174 (11)	−0.0015 (13)
C21	0.0441 (16)	0.0581 (18)	0.068 (2)	0.0082 (14)	0.0211 (14)	−0.0037 (15)
C22	0.051 (2)	0.070 (2)	0.111 (3)	−0.0021 (17)	0.024 (2)	−0.020 (2)
C23	0.0415 (19)	0.116 (4)	0.112 (4)	0.010 (2)	0.008 (2)	−0.048 (3)
C24	0.049 (2)	0.148 (5)	0.059 (2)	0.032 (3)	−0.0014 (16)	−0.021 (3)
C25	0.0470 (17)	0.098 (3)	0.0527 (18)	0.0202 (18)	0.0141 (14)	0.0052 (18)
N1	0.0420 (12)	0.0391 (11)	0.0415 (11)	0.0061 (9)	0.0155 (9)	0.0025 (9)
N2	0.0544 (15)	0.0668 (17)	0.0552 (15)	0.0032 (13)	0.0283 (12)	0.0068 (13)
O1	0.0772 (15)	0.0467 (12)	0.0726 (14)	0.0203 (11)	0.0439 (12)	0.0080 (10)

O2	0.0696 (14)	0.0626 (13)	0.0396 (10)	0.0056 (11)	0.0249 (10)	−0.0039 (9)
S1	0.0508 (4)	0.0455 (4)	0.0419 (4)	0.0091 (3)	0.0230 (3)	0.0002 (3)

Geometric parameters (Å, º)

C1—C6	1.389 (4)	C14—H14	0.9300
C1—C2	1.392 (4)	C15—C16	1.390 (5)
C1—N1	1.435 (3)	C15—H15	0.9300
C2—C3	1.379 (4)	C16—C17	1.364 (5)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.387 (5)	C17—C18	1.403 (4)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.372 (4)	C18—N2	1.390 (4)
C4—H4	0.9300	C19—N2	1.297 (4)
C5—C6	1.388 (4)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.387 (4)
C6—C7	1.444 (4)	C20—C25	1.393 (4)
C7—C8	1.376 (4)	C20—S1	1.750 (3)
C7—C12	1.409 (3)	C21—C22	1.384 (5)
C8—C9	1.400 (4)	C21—H21	0.9300
C8—H8	0.9300	C22—C23	1.364 (6)
C9—C10	1.415 (3)	C22—H22	0.9300
C9—C19	1.435 (4)	C23—C24	1.381 (7)
C10—C11	1.407 (3)	C23—H23	0.9300
C10—C13	1.450 (3)	C24—C25	1.388 (6)
C11—C12	1.379 (3)	C24—H24	0.9300
C11—H11	0.9300	C25—H25	0.9300
C12—N1	1.426 (3)	N1—S1	1.660 (2)
C13—C14	1.405 (4)	O1—S1	1.427 (2)
C13—C18	1.409 (4)	O2—S1	1.420 (2)
C14—C15	1.375 (4)		
C6—C1—C2	121.5 (3)	C14—C15—H15	119.9
C6—C1—N1	108.8 (2)	C16—C15—H15	119.9
C2—C1—N1	129.7 (3)	C17—C16—C15	119.9 (3)
C3—C2—C1	116.9 (3)	C17—C16—H16	120.0
C3—C2—H2	121.6	C15—C16—H16	120.0
C1—C2—H2	121.6	C16—C17—C18	120.9 (3)
C2—C3—C4	122.2 (3)	C16—C17—H17	119.5
C2—C3—H3	118.9	C18—C17—H17	119.5
C4—C3—H3	118.9	N2—C18—C17	116.7 (3)
C5—C4—C3	120.2 (3)	N2—C18—C13	123.4 (2)
C5—C4—H4	119.9	C17—C18—C13	119.9 (3)
C3—C4—H4	119.9	N2—C19—C9	125.2 (3)
C4—C5—C6	118.9 (3)	N2—C19—H19	117.4
C4—C5—H5	120.5	C9—C19—H19	117.4
C6—C5—H5	120.5	C21—C20—C25	121.0 (3)
C5—C6—C1	120.2 (3)	C21—C20—S1	119.5 (2)

C5—C6—C7	132.2 (3)	C25—C20—S1	119.5 (3)
C1—C6—C7	107.5 (2)	C22—C21—C20	119.3 (4)
C8—C7—C12	119.6 (2)	C22—C21—H21	120.4
C8—C7—C6	131.9 (2)	C20—C21—H21	120.4
C12—C7—C6	108.5 (2)	C23—C22—C21	120.6 (4)
C7—C8—C9	119.2 (2)	C23—C22—H22	119.7
C7—C8—H8	120.4	C21—C22—H22	119.7
C9—C8—H8	120.4	C22—C23—C24	119.9 (4)
C8—C9—C10	121.1 (2)	C22—C23—H23	120.0
C8—C9—C19	120.2 (2)	C24—C23—H23	120.0
C10—C9—C19	118.8 (2)	C23—C24—C25	121.3 (4)
C11—C10—C9	119.4 (2)	C23—C24—H24	119.4
C11—C10—C13	123.7 (2)	C25—C24—H24	119.4
C9—C10—C13	116.9 (2)	C24—C25—C20	117.9 (4)
C12—C11—C10	118.3 (2)	C24—C25—H25	121.1
C12—C11—H11	120.9	C20—C25—H25	121.1
C10—C11—H11	120.9	C12—N1—C1	107.6 (2)
C11—C12—C7	122.4 (2)	C12—N1—S1	125.03 (17)
C11—C12—N1	130.0 (2)	C1—N1—S1	123.60 (18)
C7—C12—N1	107.5 (2)	C19—N2—C18	117.3 (2)
C14—C13—C18	117.8 (2)	O2—S1—O1	120.34 (13)
C14—C13—C10	123.8 (2)	O2—S1—N1	106.19 (12)
C18—C13—C10	118.5 (2)	O1—S1—N1	106.70 (12)
C15—C14—C13	121.3 (3)	O2—S1—C20	108.65 (14)
C15—C14—H14	119.3	O1—S1—C20	108.92 (15)
C13—C14—H14	119.3	N1—S1—C20	104.97 (12)
C14—C15—C16	120.2 (3)		

C6—C1—C2—C3	1.1 (4)	C16—C17—C18—N2	−179.5 (3)
N1—C1—C2—C3	−176.1 (3)	C16—C17—C18—C13	0.5 (4)
C1—C2—C3—C4	−0.3 (5)	C14—C13—C18—N2	179.8 (3)
C2—C3—C4—C5	−0.8 (5)	C10—C13—C18—N2	0.0 (4)
C3—C4—C5—C6	1.1 (5)	C14—C13—C18—C17	−0.2 (4)
C4—C5—C6—C1	−0.3 (4)	C10—C13—C18—C17	180.0 (2)
C4—C5—C6—C7	176.9 (3)	C8—C9—C19—N2	179.1 (3)
C2—C1—C6—C5	−0.9 (4)	C10—C9—C19—N2	−0.2 (5)
N1—C1—C6—C5	176.9 (2)	C25—C20—C21—C22	−1.2 (4)
C2—C1—C6—C7	−178.7 (3)	S1—C20—C21—C22	179.9 (2)
N1—C1—C6—C7	−0.9 (3)	C20—C21—C22—C23	2.0 (5)
C5—C6—C7—C8	0.0 (5)	C21—C22—C23—C24	−1.1 (6)
C1—C6—C7—C8	177.4 (3)	C22—C23—C24—C25	−0.5 (6)
C5—C6—C7—C12	−177.5 (3)	C23—C24—C25—C20	1.2 (5)
C1—C6—C7—C12	0.0 (3)	C21—C20—C25—C24	−0.4 (4)
C12—C7—C8—C9	−1.1 (4)	S1—C20—C25—C24	178.5 (2)
C6—C7—C8—C9	−178.3 (3)	C11—C12—N1—C1	−178.7 (2)
C7—C8—C9—C10	0.6 (4)	C7—C12—N1—C1	−1.4 (3)
C7—C8—C9—C19	−178.7 (3)	C11—C12—N1—S1	22.5 (4)
C8—C9—C10—C11	0.2 (4)	C7—C12—N1—S1	−160.13 (18)

C19—C9—C10—C11	179.6 (2)	C6—C1—N1—C12	1.4 (3)
C8—C9—C10—C13	179.9 (2)	C2—C1—N1—C12	179.0 (3)
C19—C9—C10—C13	−0.8 (4)	C6—C1—N1—S1	160.52 (19)
C9—C10—C11—C12	−0.7 (4)	C2—C1—N1—S1	−21.9 (4)
C13—C10—C11—C12	179.7 (2)	C9—C19—N2—C18	1.1 (5)
C10—C11—C12—C7	0.2 (4)	C17—C18—N2—C19	179.1 (3)
C10—C11—C12—N1	177.2 (2)	C13—C18—N2—C19	−0.9 (4)
C8—C7—C12—C11	0.6 (4)	C12—N1—S1—O2	−163.8 (2)
C6—C7—C12—C11	178.5 (2)	C1—N1—S1—O2	40.7 (2)
C8—C7—C12—N1	−176.9 (2)	C12—N1—S1—O1	−34.3 (3)
C6—C7—C12—N1	0.9 (3)	C1—N1—S1—O1	170.2 (2)
C11—C10—C13—C14	0.7 (4)	C12—N1—S1—C20	81.2 (2)
C9—C10—C13—C14	−179.0 (2)	C1—N1—S1—C20	−74.3 (2)
C11—C10—C13—C18	−179.5 (2)	C21—C20—S1—O2	−19.3 (3)
C9—C10—C13—C18	0.9 (3)	C25—C20—S1—O2	161.8 (2)
C18—C13—C14—C15	0.0 (4)	C21—C20—S1—O1	−152.1 (2)
C10—C13—C14—C15	179.8 (3)	C25—C20—S1—O1	29.0 (3)
C13—C14—C15—C16	−0.1 (5)	C21—C20—S1—N1	94.0 (2)
C14—C15—C16—C17	0.4 (5)	C25—C20—S1—N1	−84.9 (2)
C15—C16—C17—C18	−0.6 (5)		

Hydrogen-bond geometry (Å, º)

*Cg*1 is the centroid of ring C13–C18 and *Cg*2 is the centroid of ring C7–C12.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2	0.93	2.36	2.944 (4)	121
C11—H11···O1	0.93	2.34	2.940 (3)	122
C21—H21···N2^{i}	0.93	2.64	3.476 (4)	150
C4—H4···*Cg*1^{ii}	0.93	2.80	3.605 (4)	145
C16—H16···*Cg*3^{iii}	0.93	2.99	3.747 (3)	139

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