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Benzyl 3-(3,4,5-trimethoxybenzylidene)dithiocarbazate

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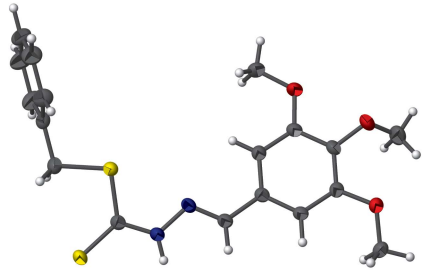
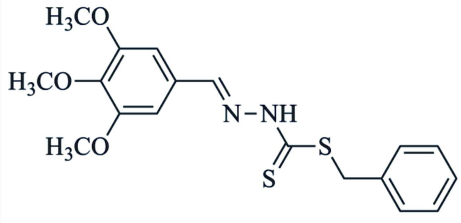
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{18}H_{20}N_2O_3S_2$, a dithiocarbazate derivative, adopts an *E* conformation about the C=N bond. The trimethoxyphenyl group and the dithiocarbazate fragment lie almost in the same plane, with the mean plane of the dithiocarbazate unit being inclined to the trimethoxyphenyl ring by 13.34 (6)°. The aromatic rings are inclined to one another by 75.30 (9)°. In the crystal, molecules are linked *via* pairs of N—H···S hydrogen bonds, forming inversion dimers with an $R_2^2(8)$ ring motif. The dimers are linked *via* C—H···O hydrogen bonds, forming undulating sheets lying parallel to (103) which are linked *via* C—H···π interactions, forming a three-dimensional supramolecular structure.

3D view



Chemical scheme



Structure description

There has been immense interest on nitrogen–sulfur donor ligands since the report on *S*-benzyldithiocarbazate (SBDTC) (Ali & Tarafder, 1977). The versatile coordination chemistry and increasingly important biological properties of ligands derived from SBDTC have also received much attention (Ali *et al.*, 2001, 2002; Crouse *et al.*, 2004, Tarafder *et al.*, 2001). The synthesis and structure of SBDTC has been reported previously (Ali & Tarafder, 1977). In a continuation of our research in this field, the title potentially bidentate (NS) Schiff base was synthesized and its crystal structure is reported on herein.

The molecular structure of the title compound is illustrated in Fig. 1. The geometric details are similar to those in two closely related compounds, namely benzyl (*E*)-3(4-

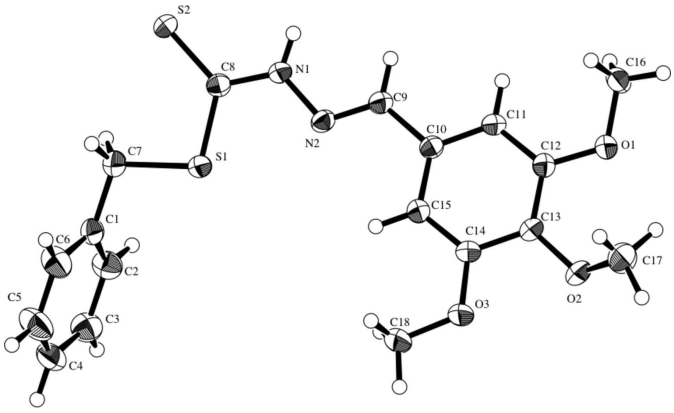


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom labelling.

methoxybenzylidene)dithiocarbazate (Fan *et al.*, 2011) and benzyl 2-(3,4-dimethoxybenzylidene)dithiocarbazate (Tan *et al.*, 2015). The essential difference being the dihedral angle between the two aromatic rings; 85.7 (3)° in the first and 65.59 (8) and 73.10 (8)° in the second compound (Z' = 2). In the title compound this dihedral angle is 75.30 (9)°.

In the crystal, inversion dimers are formed with molecules being linked *via* pairs of N—H···S hydrogen bonds (Table 1 and Fig. 2). The dimers are linked *via* C—H···O hydrogen bonds, forming undulating sheets parallel to (103); see Fig. 2 and Table 1, which in turn are linked by C—H···π interactions

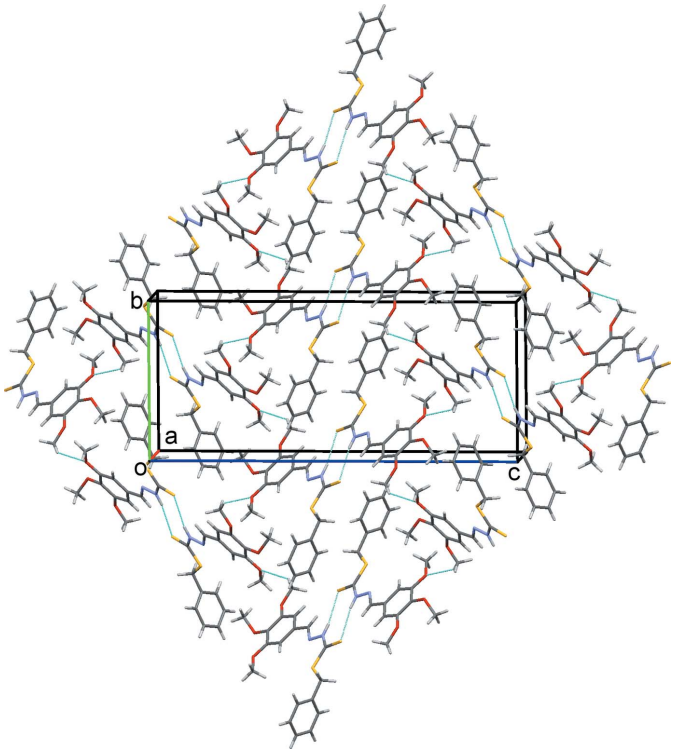


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. The hydrogen bonds are shown as dashed lines (Table 1).

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

Cg2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H8···S2^{i}	0.87 (2)	2.52 (2)	3.381 (2)	169 (2)
C16—H14···O3^{ii}	0.98	2.41	3.191 (2)	137
C18—H18···*Cg2*^{iii}	0.98	2.80	3.668 (2)	148

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

forming a three-dimensional supramolecular structure (Table 1).

Synthesis and crystallization

The ligand precursor, *S*-benzyl dithiocarbazate (SBDTC) was prepared by a literature method (Ali & Tarafder, 1977). The title Schiff base was prepared by adding the ligand precursor, SBDTC (0.99 g, 5 mmol) dissolved in ethanol (40 ml), to a solution of 3,4,5-trimethoxy benzaldehyde (0.98 g, 5 mmol) in ethanol (10 ml) and the mixture was heated under reflux for 1 h. The light yellow precipitate that formed was filtered off, washed with hot ethanol and dried under vacuum over anhydrous $CaCl_2$ (yield: 1.10 g, 56%). 175 mg of the title

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{20}N_2O_3S_2$
M_r	376.49
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	173
a, *b*, *c* (Å)	6.24258 (11), 11.4063 (2), 26.2386 (5)
β (°)	90.1171 (7)
V (Å^3)	1868.31 (6)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.75
Crystal size (mm)	0.35 × 0.28 × 0.19
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Higashi, 1995)
T_{min}, T_{max}	0.506, 0.593
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	21554, 3432, 3235
R_{int}	0.062
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.098, 1.06
No. of reflections	3432
No. of parameters	230
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.33, −0.30

Computer programs: *RAPID-AUTO* (Rigaku, 2001), *SIR92* (Altomare *et al.*, 1994), *SHELXL97* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008), *CrystalStructure* (Rigaku, 2010).

compound were dissolved in ethanol (15 ml) on warming and the resulting yellow solution was allowed to stand at room temperature for slow evaporation of the solvent. Yellow plate-like single crystals were obtained after 15 days (m.p. 431–432 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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Benzyl 3-(3,4,5-trimethoxybenzylidene)dithiocarbazate

Crystal data

$C_{18}H_{20}N_2O_3S_2$
M_r = 376.49
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.24258 (11) Å
b = 11.4063 (2) Å
c = 26.2386 (5) Å
β = 90.1171 (7)°
V = 1868.31 (6) Å^3
Z = 4
$F(000)$ = 792.00
D_x = 1.338 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 21153 reflections
θ = 3.4–68.3°
μ = 2.75 mm^{-1}
T = 173 K
Prism, colorless
0.35 × 0.28 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
T_{min} = 0.506, T_{max} = 0.593
21554 measured reflections
3432 independent reflections
3235 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.062
θ_{max} = 68.3°
h = −7→7
k = −13→13
l = −31→31

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.06
3432 reflections
230 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
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.7342P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 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 convariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; corrections 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 was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.58993 (6)	0.32030 (3)	0.572138 (14)	0.02876 (13)
S2	0.72890 (6)	0.14497 (4)	0.492037 (15)	0.03325 (14)
O1	−0.57057 (17)	−0.00200 (10)	0.68375 (4)	0.0312 (3)
O2	−0.4893 (2)	0.16929 (11)	0.75534 (5)	0.0424 (4)
O3	−0.1411 (2)	0.29687 (12)	0.75144 (5)	0.0407 (3)
N1	0.3850 (2)	0.12935 (12)	0.54866 (5)	0.0274 (3)
N2	0.2535 (2)	0.16318 (11)	0.58823 (5)	0.0260 (3)
C1	0.8673 (3)	0.50012 (15)	0.56699 (6)	0.0308 (4)
C2	0.7383 (3)	0.59440 (16)	0.55381 (7)	0.0378 (4)
C3	0.7714 (3)	0.70419 (16)	0.57498 (7)	0.0410 (5)
C4	0.9326 (3)	0.72065 (16)	0.60977 (8)	0.0430 (5)
C5	1.0614 (4)	0.62829 (18)	0.62351 (9)	0.0524 (6)
C6	1.0298 (3)	0.51833 (16)	0.60222 (8)	0.0432 (5)
C7	0.8316 (3)	0.38117 (15)	0.54361 (7)	0.0355 (4)
C8	0.5593 (3)	0.19103 (13)	0.53718 (6)	0.0257 (4)
C9	0.0923 (3)	0.09592 (13)	0.59562 (6)	0.0256 (4)
C10	−0.0568 (3)	0.11515 (13)	0.63747 (6)	0.0242 (3)
C11	−0.2397 (3)	0.04602 (13)	0.63982 (6)	0.0243 (3)
C12	−0.3865 (3)	0.06133 (13)	0.67907 (6)	0.0253 (4)
C13	−0.3489 (3)	0.14652 (14)	0.71643 (6)	0.0289 (4)
C14	−0.1638 (3)	0.21614 (14)	0.71337 (6)	0.0293 (4)
C15	−0.0170 (3)	0.20056 (14)	0.67457 (6)	0.0277 (4)
C16	−0.5848 (3)	−0.10738 (15)	0.65484 (6)	0.0337 (4)
C17	−0.5539 (4)	0.0735 (2)	0.78659 (7)	0.0519 (6)
C18	0.0391 (3)	0.37378 (17)	0.74869 (7)	0.0425 (5)
H1	0.6256	0.5835	0.5299	0.0454*
H2	0.6824	0.7681	0.5654	0.0492*
H3	0.9552	0.7959	0.6244	0.0516*
H4	1.1728	0.6398	0.6477	0.0629*
H5	1.1202	0.4550	0.6118	0.0518*
H6	0.9557	0.3295	0.5506	0.0426*
H7	0.8137	0.3883	0.5062	0.0426*
H8	0.361 (3)	0.0623 (19)	0.5340 (8)	0.034 (5)*
H9	0.0692	0.0317	0.5732	0.0308*
H10	−0.2647	−0.0120	0.6145	0.0291*
H11	0.1090	0.2471	0.6731	0.0332*
H12	−0.4516	−0.1520	0.6586	0.0404*
H13	−0.6075	−0.0882	0.6188	0.0404*
H14	−0.7053	−0.1545	0.6672	0.0404*
H15	−0.4318	0.0210	0.7922	0.0623*
H16	−0.6697	0.0304	0.7697	0.0623*

H17	−0.6046	0.1033	0.8195	0.0623*
H18	0.0294	0.4325	0.7758	0.0511*
H19	0.0403	0.4131	0.7155	0.0511*
H20	0.1713	0.3284	0.7529	0.0511*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0311 (3)	0.0264 (3)	0.0288 (3)	−0.00276 (14)	0.00610 (16)	−0.00455 (15)
S2	0.0329 (3)	0.0374 (3)	0.0295 (3)	−0.00612 (16)	0.01092 (17)	−0.00980 (16)
O1	0.0283 (6)	0.0331 (6)	0.0321 (6)	−0.0073 (5)	0.0059 (5)	−0.0062 (5)
O2	0.0412 (7)	0.0421 (7)	0.0439 (8)	−0.0058 (6)	0.0220 (6)	−0.0138 (6)
O3	0.0415 (7)	0.0441 (7)	0.0365 (7)	−0.0143 (6)	0.0117 (6)	−0.0202 (6)
N1	0.0299 (7)	0.0280 (7)	0.0243 (7)	−0.0036 (6)	0.0056 (6)	−0.0062 (6)
N2	0.0283 (7)	0.0282 (7)	0.0216 (7)	0.0010 (6)	0.0038 (5)	−0.0019 (5)
C1	0.0303 (8)	0.0288 (8)	0.0335 (9)	−0.0043 (7)	0.0060 (7)	0.0018 (7)
C2	0.0383 (10)	0.0370 (10)	0.0381 (10)	0.0012 (8)	−0.0076 (8)	−0.0010 (8)
C3	0.0447 (10)	0.0307 (9)	0.0477 (11)	0.0056 (8)	−0.0013 (9)	0.0028 (8)
C4	0.0445 (11)	0.0290 (9)	0.0554 (12)	−0.0067 (8)	−0.0010 (9)	−0.0053 (9)
C5	0.0447 (11)	0.0433 (11)	0.0691 (14)	−0.0053 (9)	−0.0210 (10)	−0.0059 (10)
C6	0.0373 (10)	0.0324 (10)	0.0598 (12)	0.0008 (8)	−0.0102 (9)	0.0036 (9)
C7	0.0327 (9)	0.0323 (9)	0.0415 (10)	−0.0056 (7)	0.0109 (8)	−0.0037 (8)
C8	0.0283 (8)	0.0290 (8)	0.0198 (7)	−0.0007 (6)	−0.0002 (6)	−0.0007 (6)
C9	0.0279 (8)	0.0256 (8)	0.0235 (8)	0.0007 (6)	0.0010 (6)	−0.0019 (6)
C10	0.0254 (8)	0.0239 (7)	0.0232 (7)	0.0025 (6)	0.0006 (6)	0.0005 (6)
C11	0.0281 (8)	0.0224 (7)	0.0223 (7)	0.0011 (6)	0.0004 (6)	−0.0015 (6)
C12	0.0234 (7)	0.0258 (8)	0.0265 (8)	−0.0003 (6)	0.0001 (6)	0.0010 (6)
C13	0.0284 (8)	0.0308 (9)	0.0275 (8)	0.0007 (7)	0.0068 (7)	−0.0047 (7)
C14	0.0311 (8)	0.0293 (8)	0.0274 (8)	−0.0020 (7)	0.0021 (7)	−0.0073 (7)
C15	0.0261 (8)	0.0294 (8)	0.0275 (8)	−0.0030 (6)	0.0018 (6)	−0.0030 (7)
C16	0.0372 (9)	0.0330 (9)	0.0310 (9)	−0.0121 (7)	0.0031 (7)	−0.0035 (7)
C17	0.0575 (13)	0.0635 (14)	0.0347 (10)	−0.0193 (11)	0.0176 (9)	−0.0105 (10)
C18	0.0431 (11)	0.0448 (11)	0.0398 (10)	−0.0144 (9)	0.0053 (8)	−0.0178 (9)

Geometric parameters (Å, º)

S1—C7	1.8229 (18)	C12—C13	1.400 (3)
S1—C8	1.7468 (16)	C13—C14	1.404 (3)
S2—C8	1.6748 (16)	C14—C15	1.383 (3)
O1—C12	1.3632 (19)	N1—H8	0.87 (2)
O1—C16	1.424 (2)	C2—H1	0.950
O2—C13	1.372 (2)	C3—H2	0.950
O2—C17	1.425 (3)	C4—H3	0.950
O3—C14	1.366 (2)	C5—H4	0.950
O3—C18	1.429 (3)	C6—H5	0.950
N1—N2	1.3798 (19)	C7—H6	0.990
N1—C8	1.331 (2)	C7—H7	0.990
N2—C9	1.281 (2)	C9—H9	0.950

C1—C2	1.387 (3)	C11—H10	0.950
C1—C6	1.387 (3)	C15—H11	0.950
C1—C7	1.505 (3)	C16—H12	0.980
C2—C3	1.385 (3)	C16—H13	0.980
C3—C4	1.370 (3)	C16—H14	0.980
C4—C5	1.373 (3)	C17—H15	0.980
C5—C6	1.387 (3)	C17—H16	0.980
C9—C10	1.457 (3)	C17—H17	0.980
C10—C11	1.389 (2)	C18—H18	0.980
C10—C15	1.399 (3)	C18—H19	0.980
C11—C12	1.391 (3)	C18—H20	0.980

S1···N2	2.7936 (14)	C16···H9^{iv}	3.4278
S1···C2	3.2963 (19)	C16···H17^{iii}	3.5696
S2···C7	3.0818 (18)	C16···H18^{iii}	3.3523
O1···O2	2.7567 (17)	C17···H4^{x}	3.0305
O1···C17	2.834 (3)	C17···H12^{v}	3.4452
O2···O3	2.6179 (19)	C17···H19^{iii}	3.5451
N2···C15	2.860 (2)	C17···H20^{iv}	3.4889
C1···C4	2.784 (3)	C18···H3^{x}	3.4471
C2···C5	2.747 (3)	C18···H12^{vii}	3.5514
C3···C6	2.757 (3)	C18···H14^{v}	3.0549
C8···C9	3.471 (3)	C18···H15^{vii}	3.1606
C10···C13	2.786 (3)	C18···H16^{v}	2.9559
C11···C14	2.777 (3)	H1···S1^{viii}	3.1884
C11···C16	2.804 (3)	H1···C7^{viii}	3.4647
C12···C15	2.803 (3)	H1···C8^{viii}	3.3216
C12···C17	3.014 (3)	H1···H1^{viii}	2.9226
C14···C17	3.505 (3)	H1···H6^{xi}	3.5063
C15···C18	2.794 (3)	H1···H7^{viii}	2.9175
S2···N1^{i}	3.3813 (15)	H2···S2^{viii}	3.1351
S2···C9^{ii}	3.5806 (16)	H2···N1^{viii}	3.2393
O1···O3^{iii}	3.3774 (18)	H2···C8^{viii}	3.1173
O1···N2^{iv}	3.3205 (17)	H2···C16^{xii}	3.2138
O1···C9^{iv}	3.3173 (19)	H2···H8^{viii}	3.2579
O1···C10^{iv}	3.5294 (18)	H2···H10^{xii}	2.8401
O2···C16^{v}	3.500 (2)	H2···H12^{xii}	2.7423
O3···O1^{v}	3.3774 (18)	H2···H13^{xii}	2.8181
O3···C16^{v}	3.191 (2)	H2···H17^{vii}	3.5924
N1···S2^{i}	3.3813 (15)	H3···O3^{xiv}	3.4567
N1···C11^{ii}	3.477 (2)	H3···C11^{xii}	3.1286
N2···O1^{ii}	3.3205 (17)	H3···C16^{xiii}	3.1770
N2···C12^{ii}	3.473 (2)	H3···C18^{xiv}	3.4471
C8···C11^{ii}	3.398 (3)	H3···H9^{xii}	3.0905
C9···S2^{iv}	3.5806 (16)	H3···H10^{xii}	2.5989
C9···O1^{ii}	3.3173 (19)	H3···H12^{xii}	2.7598
C9···C16^{ii}	3.441 (3)	H3···H13^{xiii}	3.0378
C10···O1^{ii}	3.5294 (18)	H3···H14^{xiii}	2.4634

C11···N1^{iv}	3.477 (2)	H3···H17^{vii}	3.4347
C11···C8^{iv}	3.398 (3)	H3···H18^{xiv}	3.0487
C12···N2^{iv}	3.473 (2)	H3···H20^{xiv}	3.3387
C12···C18^{vi}	3.585 (3)	H4···O2^{xiv}	3.2350
C16···O2^{iii}	3.500 (2)	H4···O3^{xiv}	3.2021
C16···O3^{iii}	3.191 (2)	H4···C16^{xiii}	3.2619
C16···C9^{iv}	3.441 (3)	H4···C17^{xiv}	3.0305
C18···C12^{vii}	3.585 (3)	H4···H12^{xiii}	3.3486
S1···H1	3.2085	H4···H13^{xiii}	3.4773
S1···H8	3.42 (2)	H4···H14^{xiii}	2.5194
S2···H6	2.9641	H4···H15^{xiv}	2.6321
S2···H7	2.8496	H4···H17^{xiv}	2.8585
S2···H8	2.72 (2)	H4···H19^{ii}	3.2460
O1···H10	2.6408	H5···S1^{ii}	3.4726
O1···H15	2.9831	H5···N2^{ii}	3.4872
O1···H16	2.3678	H5···C15^{ii}	3.4458
O3···H11	2.6448	H5···H11^{ii}	2.8662
N1···H9	2.3550	H5···H15^{xiv}	3.2679
N2···H11	2.5887	H5···H19^{ii}	2.8073
C1···H2	3.2671	H6···N1^{ii}	3.5208
C1···H4	3.2629	H6···N2^{ii}	2.8329
C2···H3	3.2452	H6···C2^{xi}	3.4527
C2···H5	3.2422	H6···C9^{ii}	3.0365
C2···H6	3.3133	H6···C10^{ii}	3.3446
C2···H7	2.7037	H6···C15^{ii}	3.5747
C3···H4	3.2316	H6···H1^{xi}	3.5063
C4···H1	3.2396	H6···H9^{ii}	3.5202
C4···H5	3.2486	H6···H11^{ii}	3.4827
C5···H2	3.2332	H7···C1^{xi}	3.0486
C6···H1	3.2409	H7···C2^{xi}	3.2187
C6···H3	3.2523	H7···C3^{xi}	3.5191
C6···H6	2.5858	H7···C5^{xi}	3.4992
C6···H7	3.2170	H7···C6^{xi}	3.1936
C7···H1	2.6665	H7···H1^{viii}	2.9175
C7···H5	2.6731	H7···H7^{xi}	3.4664
C8···H6	2.9563	H8···S2^{i}	2.52 (2)
C8···H7	2.8719	H8···N1^{i}	3.47 (2)
C9···H8	2.36 (2)	H8···C8^{i}	3.48 (2)
C9···H10	2.5943	H8···H2^{viii}	3.2579
C9···H11	2.6686	H8···H8^{i}	2.87 (3)
C11···H9	2.6104	H8···H10^{ii}	3.2598
C11···H11	3.2801	H8···H13^{ii}	2.8170
C11···H12	2.6643	H9···S2^{iv}	3.2710
C11···H13	2.8124	H9···S2^{i}	2.9309
C12···H12	2.5252	H9···C16^{ii}	3.4278
C12···H13	2.7018	H9···H3^{xv}	3.0905
C12···H14	3.1803	H9···H6^{iv}	3.5202
C12···H15	3.0164	H9···H13^{ii}	2.7142

C12···H16	2.9863	H9···H14^{ii}	3.5445
C13···H10	3.2712	H10···N1^{iv}	3.2172
C13···H11	3.2851	H10···C3^{xv}	3.4074
C13···H15	2.5039	H10···C4^{xv}	3.2917
C13···H16	2.7799	H10···C8^{iv}	3.2674
C13···H17	3.1809	H10···H2^{xv}	2.8401
C14···H15	3.4698	H10···H3^{xv}	2.5989
C14···H18	3.1977	H10···H8^{iv}	3.2598
C14···H19	2.5834	H10···H18^{vi}	3.2894
C14···H20	2.6612	H11···O1^{ii}	3.4859
C15···H9	3.3282	H11···O2^{ii}	3.4215
C15···H10	3.2774	H11···H5^{iv}	2.8662
C15···H19	2.6753	H11···H6^{iv}	3.4827
C15···H20	2.7782	H12···O2^{iii}	3.0650
C16···H10	2.5114	H12···O3^{iii}	3.5216
C16···H16	3.4400	H12···C3^{xv}	3.0744
C18···H11	2.4922	H12···C4^{xv}	3.0845
H1···H2	2.3281	H12···C17^{iii}	3.4452
H1···H6	3.5962	H12···C18^{vi}	3.5514
H1···H7	2.5940	H12···H2^{xv}	2.7423
H2···H3	2.3210	H12···H3^{xv}	2.7598
H3···H4	2.3212	H12···H4^{xvi}	3.3486
H4···H5	2.3311	H12···H17^{iii}	2.8711
H5···H6	2.3833	H12···H18^{vi}	3.2897
H5···H7	3.4487	H12···H20^{vi}	2.9146
H8···H9	2.1210	H13···S2^{ix}	3.0738
H9···H10	2.4034	H13···N1^{iv}	3.0897
H10···H12	2.2929	H13···N2^{iv}	3.1005
H10···H13	2.3124	H13···C3^{xv}	3.5410
H10···H14	3.4837	H13···C9^{iv}	2.8789
H11···H18	3.4621	H13···H2^{xv}	2.8181
H11···H19	2.2374	H13···H3^{xvi}	3.0378
H11···H20	2.3203	H13···H4^{xvi}	3.4773
H14···H16	3.4230	H13···H8^{iv}	2.8170
S1···H1^{viii}	3.1884	H13···H9^{iv}	2.7142
S1···H5^{iv}	3.4726	H14···O2^{iii}	3.1039
S2···H2^{viii}	3.1351	H14···O3^{iii}	2.4062
S2···H8^{i}	2.52 (2)	H14···C4^{xvi}	3.0657
S2···H9^{ii}	3.2710	H14···C5^{xvi}	3.0935
S2···H9^{i}	2.9309	H14···C14^{iii}	3.5597
S2···H13^{ix}	3.0738	H14···C18^{iii}	3.0549
O1···H11^{iv}	3.4859	H14···H3^{xvi}	2.4634
O1···H18^{iii}	3.1461	H14···H4^{xvi}	2.5194
O1···H20^{vi}	3.5641	H14···H9^{iv}	3.5445
O2···H4^{x}	3.2350	H14···H17^{iii}	3.3907
O2···H11^{iv}	3.4215	H14···H18^{iii}	2.7060
O2···H12^{v}	3.0650	H14···H20^{iii}	3.5948
O2···H14^{v}	3.1039	H15···C5^{x}	3.4234

O2···H20^{iv}	2.7905	H15···C18^{vi}	3.1606
O3···H3^{x}	3.4567	H15···H4^{x}	2.6321
O3···H4^{x}	3.2021	H15···H5^{x}	3.2679
O3···H12^{v}	3.5216	H15···H18^{vi}	3.2450
O3···H14^{v}	2.4062	H15···H19^{vi}	2.7444
O3···H16^{v}	2.9656	H15···H20^{vi}	2.9788
N1···H2^{viii}	3.2393	H16···O3^{iii}	2.9656
N1···H6^{iv}	3.5208	H16···C18^{iii}	2.9559
N1···H8^{i}	3.47 (2)	H16···H18^{iii}	2.7751
N1···H10^{ii}	3.2172	H16···H19^{iii}	2.7012
N1···H13^{ii}	3.0897	H16···H20^{iv}	3.5682
N2···H5^{iv}	3.4872	H17···C2^{vi}	3.4315
N2···H6^{iv}	2.8329	H17···C3^{vi}	3.1767
N2···H13^{ii}	3.1005	H17···C4^{vi}	3.0736
C1···H7^{xi}	3.0486	H17···C5^{vi}	3.2357
C2···H6^{xi}	3.4527	H17···C6^{vi}	3.4971
C2···H7^{xi}	3.2187	H17···C16^{v}	3.5696
C2···H17^{vii}	3.4315	H17···H2^{vi}	3.5924
C3···H7^{xi}	3.5191	H17···H3^{vi}	3.4347
C3···H10^{xii}	3.4074	H17···H4^{x}	2.8585
C3···H12^{xii}	3.0744	H17···H12^{v}	2.8711
C3···H13^{xii}	3.5410	H17···H14^{v}	3.3907
C3···H17^{vii}	3.1767	H17···H19^{iii}	3.5960
C4···H10^{xii}	3.2917	H17···H20^{iv}	3.4050
C4···H12^{xii}	3.0845	H18···O1^{v}	3.1461
C4···H14^{xiii}	3.0657	H18···C10^{vii}	3.0889
C4···H17^{vii}	3.0736	H18···C11^{vii}	2.8786
C5···H7^{xi}	3.4992	H18···C12^{vii}	2.9183
C5···H14^{xiii}	3.0935	H18···C13^{vii}	3.1582
C5···H15^{xiv}	3.4234	H18···C14^{vii}	3.3538
C5···H17^{vii}	3.2357	H18···C15^{vii}	3.3236
C5···H19^{ii}	3.4448	H18···C16^{v}	3.3523
C6···H7^{xi}	3.1936	H18···H3^{x}	3.0487
C6···H17^{vii}	3.4971	H18···H10^{vii}	3.2894
C6···H19^{ii}	3.2057	H18···H12^{vii}	3.2897
C7···H1^{viii}	3.4647	H18···H14^{v}	2.7060
C8···H1^{viii}	3.3216	H18···H15^{vii}	3.2450
C8···H2^{viii}	3.1173	H18···H16^{v}	2.7751
C8···H8^{i}	3.48 (2)	H19···C5^{iv}	3.4448
C8···H10^{ii}	3.2674	H19···C6^{iv}	3.2057
C9···H6^{iv}	3.0365	H19···C17^{v}	3.5451
C9···H13^{ii}	2.8789	H19···H4^{iv}	3.2460
C10···H6^{iv}	3.3446	H19···H5^{iv}	2.8073
C10···H18^{vi}	3.0889	H19···H15^{vii}	2.7444
C11···H3^{xv}	3.1286	H19···H16^{v}	2.7012
C11···H18^{vi}	2.8786	H19···H17^{v}	3.5960
C12···H18^{vi}	2.9183	H20···O1^{vii}	3.5641
C12···H20^{vi}	3.4701	H20···O2^{ii}	2.7905

C13···H18^{vi}	3.1582	H20···C12^{vii}	3.4701
C14···H14^{v}	3.5597	H20···C17^{ii}	3.4889
C14···H18^{vi}	3.3538	H20···H3^{x}	3.3387
C15···H5^{iv}	3.4458	H20···H12^{vii}	2.9146
C15···H6^{iv}	3.5747	H20···H14^{v}	3.5948
C15···H18^{vi}	3.3236	H20···H15^{vii}	2.9788
C16···H2^{xv}	3.2138	H20···H16^{ii}	3.5682
C16···H3^{xvi}	3.1770	H20···H17^{ii}	3.4050
C16···H4^{xvi}	3.2619		

C7—S1—C8	101.28 (8)	C2—C3—H2	120.003
C12—O1—C16	116.82 (12)	C4—C3—H2	120.015
C13—O2—C17	117.73 (15)	C3—C4—H3	120.045
C14—O3—C18	117.24 (14)	C5—C4—H3	120.035
N2—N1—C8	120.69 (13)	C4—C5—H4	119.829
N1—N2—C9	114.53 (13)	C6—C5—H4	119.825
C2—C1—C6	118.27 (16)	C1—C6—H5	119.752
C2—C1—C7	120.79 (15)	C5—C6—H5	119.769
C6—C1—C7	120.93 (16)	S1—C7—H6	110.240
C1—C2—C3	121.00 (17)	S1—C7—H7	110.252
C2—C3—C4	119.98 (18)	C1—C7—H6	110.244
C3—C4—C5	119.92 (18)	C1—C7—H7	110.254
C4—C5—C6	120.3 (2)	H6—C7—H7	108.526
C1—C6—C5	120.48 (18)	N2—C9—H9	119.100
S1—C7—C1	107.33 (12)	C10—C9—H9	119.090
S1—C8—S2	124.58 (10)	C10—C11—H10	119.857
S1—C8—N1	114.58 (12)	C12—C11—H10	119.853
S2—C8—N1	120.84 (12)	C10—C15—H11	120.507
N2—C9—C10	121.81 (14)	C14—C15—H11	120.505
C9—C10—C11	118.31 (14)	O1—C16—H12	109.465
C9—C10—C15	121.09 (14)	O1—C16—H13	109.476
C11—C10—C15	120.61 (15)	O1—C16—H14	109.460
C10—C11—C12	120.29 (14)	H12—C16—H13	109.474
O1—C12—C11	123.84 (14)	H12—C16—H14	109.472
O1—C12—C13	116.42 (14)	H13—C16—H14	109.481
C11—C12—C13	119.74 (14)	O2—C17—H15	109.473
O2—C13—C12	123.10 (14)	O2—C17—H16	109.471
O2—C13—C14	117.55 (14)	O2—C17—H17	109.471
C12—C13—C14	119.30 (15)	H15—C17—H16	109.469
O3—C14—C13	115.07 (14)	H15—C17—H17	109.466
O3—C14—C15	123.85 (15)	H16—C17—H17	109.477
C13—C14—C15	121.07 (15)	O3—C18—H18	109.471
C10—C15—C14	118.99 (15)	O3—C18—H19	109.469
N2—N1—H8	118.4 (13)	O3—C18—H20	109.466
C8—N1—H8	120.5 (13)	H18—C18—H19	109.475
C1—C2—H1	119.507	H18—C18—H20	109.476
C3—C2—H1	119.494	H19—C18—H20	109.470

C7—S1—C8—S2	2.22 (13)	C3—C4—C5—C6	0.2 (3)
C7—S1—C8—N1	−177.12 (11)	C4—C5—C6—C1	−0.3 (3)
C8—S1—C7—C1	174.88 (10)	N2—C9—C10—C11	173.37 (13)
C16—O1—C12—C11	16.4 (2)	N2—C9—C10—C15	−6.9 (3)
C16—O1—C12—C13	−164.06 (12)	C9—C10—C11—C12	−179.97 (12)
C17—O2—C13—C12	54.5 (2)	C9—C10—C15—C14	179.56 (13)
C17—O2—C13—C14	−128.19 (15)	C11—C10—C15—C14	−0.7 (3)
C18—O3—C14—C13	−177.01 (13)	C15—C10—C11—C12	0.3 (3)
C18—O3—C14—C15	4.0 (3)	C10—C11—C12—O1	179.28 (13)
N2—N1—C8—S1	−5.15 (19)	C10—C11—C12—C13	−0.2 (3)
N2—N1—C8—S2	175.48 (11)	O1—C12—C13—O2	−1.7 (3)
C8—N1—N2—C9	−179.43 (12)	O1—C12—C13—C14	−178.96 (12)
N1—N2—C9—C10	176.75 (12)	C11—C12—C13—O2	177.85 (13)
C2—C1—C6—C5	−0.0 (3)	C11—C12—C13—C14	0.6 (3)
C6—C1—C2—C3	0.4 (3)	O2—C13—C14—O3	2.5 (2)
C2—C1—C7—S1	−73.33 (18)	O2—C13—C14—C15	−178.45 (13)
C7—C1—C2—C3	−179.58 (14)	C12—C13—C14—O3	179.90 (13)
C6—C1—C7—S1	106.70 (17)	C12—C13—C14—C15	−1.0 (3)
C7—C1—C6—C5	179.95 (15)	O3—C14—C15—C10	−179.93 (13)
C1—C2—C3—C4	−0.5 (3)	C13—C14—C15—C10	1.1 (3)
C2—C3—C4—C5	0.1 (3)		

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) −*x*−1, *y*−1/2, −*z*+3/2; (iv) *x*−1, *y*, *z*; (v) −*x*−1, *y*+1/2, −*z*+3/2; (vi) −*x*, *y*−1/2, −*z*+3/2; (vii) −*x*, *y*+1/2, −*z*+3/2; (viii) −*x*+1, −*y*+1, −*z*+1; (ix) −*x*, −*y*, −*z*+1; (x) −*x*+1, *y*−1/2, −*z*+3/2; (xi) −*x*+2, −*y*+1, −*z*+1; (xii) *x*+1, *y*+1, *z*; (xiii) *x*+2, *y*+1, *z*; (xiv) −*x*+1, *y*+1/2, −*z*+3/2; (xv) *x*−1, *y*−1, *z*; (xvi) *x*−2, *y*−1, *z*.

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C10–C15 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H8···S2^{i}	0.87 (2)	2.52 (2)	3.381 (2)	169 (2)
C16—H14···O3^{iii}	0.98	2.41	3.191 (2)	137
C18—H18···*Cg*2^{vii}	0.98	2.80	3.668 (2)	148

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