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Crystal structure of benzyl (*E*)-2-(3,4-dimethoxybenzylidene)hydrazine-1-carbodithioate

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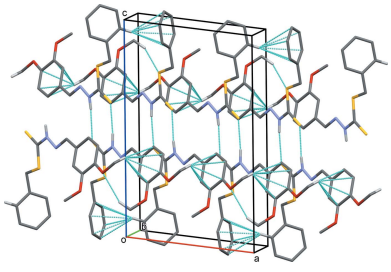
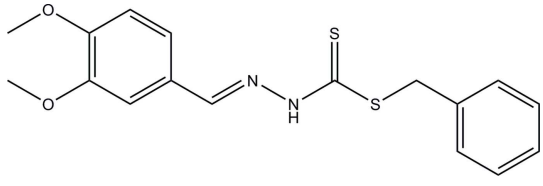
The title compound, $C_{17}H_{18}N_2O_2S_2$, synthesized *via* a condensation reaction between *S*-benzyl dithiocarbazate and 3,4-dimethoxybenzaldehyde, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. Both molecules have an L-shape but differ in the orientation of the benzyl ring with respect to the 3,4-dimethoxybenzylidine ring, this dihedral angle is 65.59 (8)° in molecule *A* and 73.10 (8)° in molecule *B*. In the crystal, the *A* and *B* molecules are linked *via* pairs of N—H···S hydrogen bonds, forming dimers with an $R_2^2(8)$ ring motif. The dimers are linked *via* pairs of C—H···O hydrogen bonds, giving inversion dimers of dimers. These units are linked by C—H···π interactions, forming ribbons propagating in the [100] direction.

1. Chemical context

Schiff bases have been proven to possess a variety of biological activities, and this has led to extensive studies on this group of compounds with particular emphasis on those derived from dithiocarbazates. Dithiocarbazate-derived Schiff bases have generally been found to exhibit interesting cytotoxic and antimicrobial activities. One of the most investigated dithiocarbazates has been *S*-benzyldithiocarbazate (SBDTC) whose derivatives have shown promising biological activities (Break *et al.*, 2013). Therefore, as part of our research which is aimed at developing anticancer and antimicrobial drugs, we have synthesized a novel Schiff base *via* the condensation reaction of SBDTC and 3,4-dimethoxybenzaldehyde. We report herein on the synthesis and crystal structure of the title compound.





2. Structural commentary

The title compound, Fig. 1, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. Both molecules have an L-shape but differ in the orientation of the benzyl ring with respect to the 3,4-dimethoxybenzylidine ring, this dihedral angle being 65.59 (8) ° in molecule *A* and 73.10 (8) ° in molecule *B* (Fig. 2).

The C—N and N(H)—C bond lengths (C1—N1 and N2—C9 in *A*, and C21—N21 and N22—C29 in *B*) are 1.331 (2) and

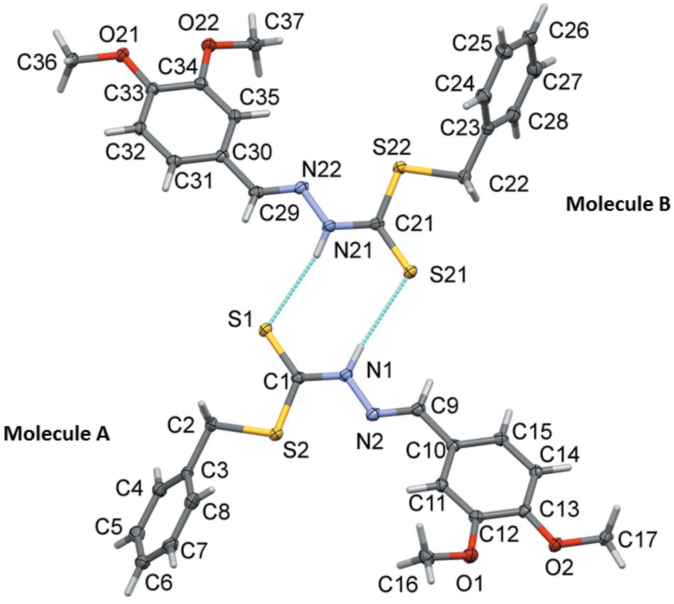


Figure 1
A view of the molecular structure of the two independent molecules (*A* and *B*) of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level. N—H···S hydrogen bonds are shown as dashed lines (see Table 1 for details).

1.282 (2) Å, respectively, in molecule *A*, and 1.336 (2) and 1.280 (2) Å, respectively, in molecule *B*. The shorter length of the C—N bond suggests the existence of a double bond which belongs to the imine group. Similarly, the shorter C—S bond length [C1—S1 = 1.681 (2) Å in *A*, and C21—S21 = 1.677 (2) Å in *B*] relative to that of [C1—S2 = 1.749 (2) Å in *A*, and C21—S22 = 1.749 (2) Å in *B*] suggests that the former possesses double-bond character, indicating that the molecule exists in its thione form in the solid state. The functional group identities proposed from these bond lengths are further supported by data obtained from the IR analysis reported below. Furthermore, the bond distances in the title compound are similar to those found for other carbodithioate-derived Schiff bases (Break *et al.*; 2013; Khoo *et al.*, 2014).

Both molecules (*A* and *B*) crystallizes in the conformer in which the two aromatic rings of the compound are *cis* with respect to each other across the C=N bonds, while the thione sulfur atom is *trans* with respect to the same bond.

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

*Cg*1, *Cg*2 and *Cg*4 are the centroids of the C3–C8, C10–C15 and C30–C35 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···S21	0.92	2.52	3.418 (1)	166
N21—H1···S1	0.87	2.55	3.407 (1)	168
C16—H163···O21^{i}	0.97	2.69	3.560 (2)	149
C17—H172···*Cg*4^{ii}	0.97	2.74	3.5587 (18)	143
C28—H281···*Cg*1^{ii}	0.94	2.94	3.6082 (18)	130
C36—H363···*Cg*2^{i}	0.97	2.67	3.5023 (17)	145

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

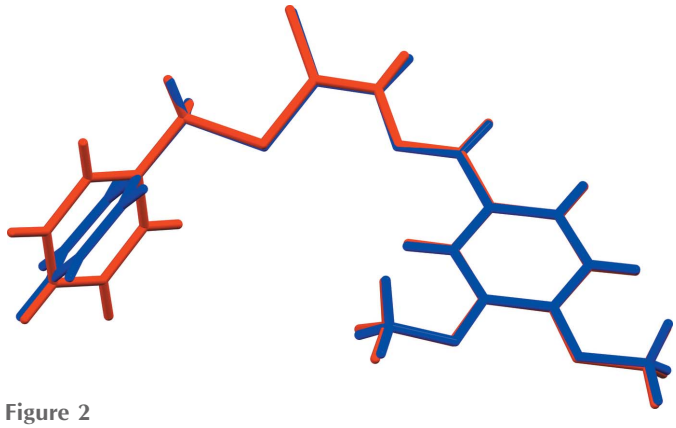


Figure 2
A view of the molecular overlay (Mercury; Macrae *et al.*, 2008) of the two independent molecules (*A* blue and *B* red) of the title compound.

3. Supramolecular features

In the crystal, the *A* and *B* molecules are linked by pairs of N—H···S hydrogen bonds, forming dimers with an R_2^2 (8) ring motif (Table 1 and Fig. 3). The dimers are linked *via* pairs of C—H···O hydrogen bonds, giving inversion dimers of dimers. These units are linked by C—H···π interactions, forming ribbons propagating in the [100] direction (Fig. 3 and Table 1).

4. Database survey

A search of the Cambridge Structural Database (Version 5.35, May 2014; Groom & Allen, 2014) for benzyl (*E*)-2-benzylidenehydrazine-1-carbodithioates gave 13 hits. One of these concerns a structure very similar to the title compound, namely benzyl (*E*)-2-(4-methoxybenzylidene)hydrazine-1-carbodithioate (YAHDAO; Fan *et al.*, 2011). Here the two aromatic rings are inclined to one another by *ca* 85.71°, compared with 65.59 (8)° in molecule *A* and 73.10 (8)° in molecule *B* of the title compound.

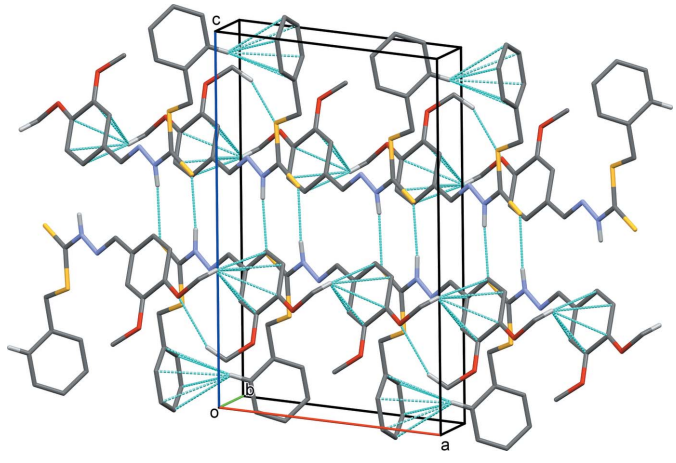


Figure 3
A view approximately along the *b* axis of the crystal structure of the title compound. The hydrogen bonds and C—H···π interactions are shown as dashed lines (see Table 1 for details; for clarity only the H atoms involved in these interactions are shown).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}N_2O_2S_2$
M_r	346.45
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	9.6432 (5), 10.796 (1), 16.1673 (10)
α, β, γ (°)	90.899 (6), 97.203 (5), 91.200 (6)
V (Å^3)	1669.2 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.98
Crystal size (mm)	0.15 × 0.06 × 0.04
Data collection	
Diffractometer	Oxford Diffraction Gemini
Absorption correction	Multi-scan (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min}, T_{max}	0.74, 0.89
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23678, 6592, 5514
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.622
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.106, 0.99
No. of reflections	6567
No. of parameters	415
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.33

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2002), *SUPERFLIP* (Palatinus & Chapuis, 2007), *CRYSTALS* (Betteridge *et al.*, 2003), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

5. Synthesis and crystallization

1.98 g (0.01 mol) of *S*-benzyldithiocarbazate in 30 ml of absolute ethanol was added to an equimolar quantity of 3,4-dimethoxybenzaldehyde in 10 ml of absolute ethanol, followed by the addition of 2–4 drops of concentrated H_2SO_4. The mixture was heated over a steam bath for 15 min and a precipitate started to form. The Schiff base which precipitated was filtered, washed with cold ethanol and dried *in vacuo* over silica gel, giving a white yellowish product. Yellow crystals of the title compound, suitable for X-ray analysis, were obtained by slow evaporation of a solution in DMSO over a period of three weeks (yield 60%; m.p. 438–439 K). IR (KBr, cm^{-1}): 3360, 3122, 1602, 1069, 1023, 950, 788, 695. LCMS (ESI$^+$): 347.1 $[M+H]^+$.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms were all located in a difference Fourier map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98 Å, N—H in the range 0.86–0.89 Å), with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and = 1.2U_{eq}(C) for other H atoms.

Acknowledgements

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supporting information

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Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED* (Oxford Diffraction, 2002); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Benzyl (*E*)-2-(3,4-dimethoxybenzylidene)hydrazine-1-carbodithioate

Crystal data

$C_{17}H_{18}N_2O_2S_2$
M_r = 346.45
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.6432 (5) Å
b = 10.796 (1) Å
c = 16.1673 (10) Å
α = 90.899 (6)°
β = 97.203 (5)°
γ = 91.200 (6)°
V = 1669.2 (2) Å^3
Z = 4
$F(000)$ = 728
D_x = 1.379 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54180 Å
Cell parameters from 8676 reflections
θ = 4–73°
μ = 2.98 mm^{-1}
T = 100 K
Plate, yellow
0.15 × 0.06 × 0.04 mm

Data collection

Oxford Diffraction Gemini diffractometer
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2002)
T_{min} = 0.74, T_{max} = 0.89
23678 measured reflections
6592 independent reflections
5514 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 73.4°, θ_{min} = 4.1°
h = −11→11
k = −13→11
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.106
S = 0.99
6567 reflections
415 parameters
0 restraints
Primary atom site location: other
Hydrogen site location: difference Fourier map
H-atom parameters constrained
Method = Modified Sheldrick $w = 1/[\sigma^2(F^2) + (0.07P)^2 + 0.48P]$, where $P = (\max(F_o^2,0) + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems open-flow nitrogen cryostat (Cosier & Glazer, 1986) with a nominal stability of 0.1K.
Cosier, J. & Glazer, A.M., 1986. J. Appl. Cryst. 105-107.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.67401 (4)	0.61670 (4)	0.39922 (2)	0.0170
C1	0.77157 (15)	0.52035 (14)	0.34926 (9)	0.0150
S2	0.78189 (4)	0.51826 (4)	0.24198 (2)	0.0182
C2	0.66277 (16)	0.64058 (15)	0.20558 (10)	0.0187
C3	0.68192 (15)	0.66561 (15)	0.11569 (9)	0.0174
C8	0.65456 (17)	0.57319 (16)	0.05415 (10)	0.0215
C7	0.67331 (17)	0.59709 (17)	−0.02786 (10)	0.0245
C6	0.71768 (17)	0.71377 (18)	−0.04941 (10)	0.0243
C5	0.74303 (17)	0.80681 (17)	0.01141 (10)	0.0239
C4	0.72699 (16)	0.78255 (16)	0.09388 (10)	0.0199
N1	0.85201 (13)	0.43802 (12)	0.39143 (8)	0.0163
N2	0.92928 (13)	0.35596 (12)	0.35025 (8)	0.0171
C9	1.01861 (16)	0.29639 (15)	0.39886 (10)	0.0171
C10	1.10446 (16)	0.20035 (14)	0.36811 (9)	0.0156
C15	1.20578 (16)	0.14725 (15)	0.42490 (10)	0.0167
C14	1.28967 (15)	0.05382 (15)	0.39928 (9)	0.0159
C13	1.27152 (15)	0.01212 (14)	0.31724 (10)	0.0154
O2	1.34580 (11)	−0.07889 (11)	0.28523 (7)	0.0187
C17	1.44520 (17)	−0.14133 (16)	0.34241 (10)	0.0204
C12	1.16634 (16)	0.06392 (15)	0.25933 (9)	0.0168
C11	1.08539 (16)	0.15789 (15)	0.28466 (10)	0.0169
O1	1.15407 (12)	0.01059 (11)	0.18189 (7)	0.0235
C16	1.03032 (18)	0.03484 (18)	0.12691 (10)	0.0242
S21	0.84603 (4)	0.37456 (4)	0.59742 (2)	0.0167
C21	0.74525 (15)	0.46870 (14)	0.64640 (9)	0.0153
S22	0.73586 (4)	0.47065 (4)	0.75377 (2)	0.0186
C22	0.84857 (16)	0.34265 (15)	0.78893 (10)	0.0186
C23	0.82688 (16)	0.31752 (15)	0.87789 (10)	0.0177
C28	0.92759 (17)	0.35307 (16)	0.94417 (10)	0.0218
C27	0.90523 (18)	0.32945 (16)	1.02578 (10)	0.0245
C26	0.78224 (19)	0.27209 (16)	1.04222 (10)	0.0241
C25	0.68103 (18)	0.23642 (17)	0.97647 (10)	0.0243
C24	0.70366 (17)	0.25821 (16)	0.89488 (10)	0.0219
N21	0.66212 (13)	0.54892 (12)	0.60336 (8)	0.0167
N22	0.58326 (14)	0.63039 (12)	0.64363 (8)	0.0174
C29	0.49371 (16)	0.68920 (15)	0.59483 (10)	0.0165
C30	0.40710 (15)	0.78438 (14)	0.62621 (10)	0.0156
C31	0.30524 (16)	0.83952 (15)	0.57104 (9)	0.0160
C32	0.22248 (15)	0.93261 (15)	0.59875 (9)	0.0161
C33	0.24252 (15)	0.97166 (14)	0.68106 (9)	0.0154

O21	0.17151 (11)	1.06326 (10)	0.71518 (7)	0.0186
C36	0.07068 (16)	1.12784 (15)	0.65980 (10)	0.0198
C34	0.34780 (16)	0.91696 (15)	0.73749 (9)	0.0165
C35	0.42769 (16)	0.82408 (15)	0.71021 (9)	0.0169
O22	0.36178 (12)	0.96604 (11)	0.81611 (7)	0.0226
C37	0.48390 (17)	0.93340 (17)	0.86989 (10)	0.0229
H21	0.6844	0.7164	0.2396	0.0224*
H22	0.5671	0.6108	0.2095	0.0226*
H81	0.6251	0.4926	0.0696	0.0260*
H71	0.6559	0.5360	−0.0684	0.0289*
H61	0.7301	0.7280	−0.1055	0.0281*
H51	0.7718	0.8866	−0.0041	0.0283*
H41	0.7470	0.8439	0.1359	0.0224*
H91	1.0307	0.3132	0.4569	0.0196*
H151	1.2192	0.1755	0.4814	0.0193*
H141	1.3600	0.0204	0.4383	0.0195*
H171	1.4887	−0.2006	0.3096	0.0295*
H172	1.5153	−0.0849	0.3703	0.0296*
H173	1.3961	−0.1841	0.3835	0.0292*
H111	1.0173	0.1922	0.2457	0.0203*
H161	1.0275	−0.0232	0.0825	0.0339*
H162	1.0336	0.1188	0.1071	0.0348*
H163	0.9479	0.0253	0.1552	0.0344*
H221	0.9453	0.3651	0.7838	0.0209*
H222	0.8212	0.2696	0.7549	0.0213*
H281	1.0106	0.3923	0.9334	0.0253*
H271	0.9755	0.3524	1.0704	0.0279*
H261	0.7688	0.2572	1.0983	0.0275*
H251	0.5958	0.1972	0.9872	0.0282*
H241	0.6357	0.2334	0.8499	0.0246*
H291	0.4816	0.6724	0.5376	0.0190*
H311	0.2919	0.8124	0.5145	0.0188*
H321	0.1533	0.9669	0.5598	0.0183*
H361	0.0297	1.1869	0.6942	0.0279*
H362	0.1185	1.1706	0.6193	0.0275*
H363	0.0006	1.0703	0.6330	0.0275*
H351	0.4958	0.7869	0.7466	0.0208*
H371	0.4800	0.9831	0.9202	0.0331*
H372	0.5668	0.9527	0.8439	0.0323*
H373	0.4801	0.8448	0.8807	0.0322*
H1	0.6713	0.5556	0.5505	0.0500*
H2	0.8546	0.4361	0.4487	0.0500*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01948 (19)	0.0154 (2)	0.01721 (19)	0.00548 (15)	0.00564 (14)	0.00046 (14)
C1	0.0153 (7)	0.0141 (8)	0.0163 (7)	−0.0008 (6)	0.0044 (5)	0.0002 (6)

S2	0.0203 (2)	0.0195 (2)	0.01605 (19)	0.00695 (15)	0.00537 (14)	0.00125 (15)
C2	0.0181 (7)	0.0188 (8)	0.0198 (8)	0.0078 (6)	0.0035 (6)	0.0031 (6)
C3	0.0130 (7)	0.0213 (8)	0.0180 (7)	0.0056 (6)	0.0012 (5)	0.0007 (6)
C8	0.0185 (7)	0.0202 (8)	0.0258 (8)	0.0040 (6)	0.0022 (6)	−0.0008 (7)
C7	0.0236 (8)	0.0294 (10)	0.0202 (8)	0.0079 (7)	0.0010 (6)	−0.0066 (7)
C6	0.0198 (8)	0.0365 (10)	0.0172 (8)	0.0089 (7)	0.0032 (6)	0.0032 (7)
C5	0.0206 (8)	0.0258 (9)	0.0258 (8)	0.0035 (7)	0.0042 (6)	0.0048 (7)
C4	0.0194 (7)	0.0196 (8)	0.0206 (8)	0.0037 (6)	0.0020 (6)	−0.0019 (6)
N1	0.0182 (6)	0.0142 (7)	0.0177 (6)	0.0033 (5)	0.0064 (5)	0.0000 (5)
N2	0.0178 (6)	0.0135 (7)	0.0213 (7)	0.0013 (5)	0.0072 (5)	0.0002 (5)
C9	0.0187 (7)	0.0147 (8)	0.0189 (7)	−0.0001 (6)	0.0059 (6)	0.0008 (6)
C10	0.0154 (7)	0.0133 (8)	0.0189 (7)	−0.0012 (6)	0.0059 (6)	0.0012 (6)
C15	0.0174 (7)	0.0161 (8)	0.0167 (7)	−0.0015 (6)	0.0034 (6)	−0.0004 (6)
C14	0.0138 (7)	0.0160 (8)	0.0180 (7)	0.0000 (6)	0.0020 (5)	0.0028 (6)
C13	0.0142 (7)	0.0128 (7)	0.0201 (7)	0.0009 (6)	0.0059 (6)	0.0015 (6)
O2	0.0195 (5)	0.0177 (6)	0.0191 (5)	0.0067 (4)	0.0032 (4)	−0.0014 (4)
C17	0.0189 (8)	0.0195 (8)	0.0238 (8)	0.0068 (6)	0.0049 (6)	0.0032 (6)
C12	0.0176 (7)	0.0176 (8)	0.0156 (7)	−0.0004 (6)	0.0038 (6)	0.0003 (6)
C11	0.0159 (7)	0.0160 (8)	0.0190 (7)	0.0018 (6)	0.0027 (6)	0.0040 (6)
O1	0.0255 (6)	0.0276 (7)	0.0170 (5)	0.0088 (5)	0.0000 (4)	−0.0037 (5)
C16	0.0241 (8)	0.0318 (10)	0.0162 (8)	0.0025 (7)	−0.0003 (6)	0.0013 (7)
S21	0.01906 (19)	0.0154 (2)	0.01649 (19)	0.00483 (15)	0.00539 (14)	−0.00063 (14)
C21	0.0168 (7)	0.0135 (8)	0.0163 (7)	−0.0011 (6)	0.0058 (6)	−0.0015 (6)
S22	0.0232 (2)	0.0181 (2)	0.01609 (19)	0.00641 (16)	0.00685 (14)	0.00131 (15)
C22	0.0188 (7)	0.0184 (8)	0.0194 (8)	0.0056 (6)	0.0048 (6)	0.0033 (6)
C23	0.0195 (7)	0.0150 (8)	0.0194 (8)	0.0056 (6)	0.0049 (6)	0.0028 (6)
C28	0.0182 (8)	0.0207 (9)	0.0265 (8)	0.0040 (6)	0.0021 (6)	0.0019 (7)
C27	0.0250 (8)	0.0244 (9)	0.0230 (8)	0.0058 (7)	−0.0020 (6)	0.0001 (7)
C26	0.0309 (9)	0.0240 (9)	0.0181 (8)	0.0073 (7)	0.0048 (7)	0.0044 (7)
C25	0.0253 (8)	0.0245 (9)	0.0236 (8)	−0.0004 (7)	0.0055 (7)	0.0035 (7)
C24	0.0215 (8)	0.0234 (9)	0.0208 (8)	0.0004 (7)	0.0023 (6)	0.0009 (6)
N21	0.0193 (6)	0.0153 (7)	0.0166 (6)	0.0037 (5)	0.0069 (5)	−0.0002 (5)
N22	0.0189 (6)	0.0134 (7)	0.0217 (7)	0.0019 (5)	0.0090 (5)	0.0001 (5)
C29	0.0178 (7)	0.0157 (8)	0.0168 (7)	−0.0023 (6)	0.0056 (6)	−0.0007 (6)
C30	0.0152 (7)	0.0124 (7)	0.0202 (7)	−0.0007 (6)	0.0067 (6)	0.0014 (6)
C31	0.0176 (7)	0.0158 (8)	0.0148 (7)	−0.0020 (6)	0.0031 (6)	−0.0016 (6)
C32	0.0142 (7)	0.0169 (8)	0.0172 (7)	0.0010 (6)	0.0014 (5)	0.0027 (6)
C33	0.0148 (7)	0.0138 (8)	0.0184 (7)	0.0006 (6)	0.0047 (6)	0.0010 (6)
O21	0.0193 (5)	0.0178 (6)	0.0190 (5)	0.0068 (4)	0.0031 (4)	−0.0009 (4)
C36	0.0185 (7)	0.0173 (8)	0.0244 (8)	0.0066 (6)	0.0049 (6)	0.0038 (6)
C34	0.0185 (7)	0.0172 (8)	0.0146 (7)	−0.0001 (6)	0.0047 (6)	0.0007 (6)
C35	0.0166 (7)	0.0173 (8)	0.0171 (7)	0.0035 (6)	0.0024 (6)	0.0032 (6)
O22	0.0262 (6)	0.0276 (7)	0.0139 (5)	0.0110 (5)	0.0005 (4)	−0.0025 (5)
C37	0.0242 (8)	0.0298 (10)	0.0146 (7)	0.0055 (7)	0.0013 (6)	0.0013 (7)

Geometric parameters (Å, º)

S1—C1	1.6807 (15)	S21—C21	1.6774 (15)
C1—S2	1.7494 (15)	C21—S22	1.7494 (15)
C1—N1	1.331 (2)	C21—N21	1.336 (2)
S2—C2	1.8244 (15)	S22—C22	1.8294 (16)
C2—C3	1.516 (2)	C22—C23	1.507 (2)
C2—H21	0.983	C22—H221	0.973
C2—H22	0.980	C22—H222	0.968
C3—C8	1.395 (2)	C23—C28	1.396 (2)
C3—C4	1.392 (2)	C23—C24	1.397 (2)
C8—C7	1.388 (2)	C28—C27	1.390 (2)
C8—H81	0.956	C28—H281	0.935
C7—C6	1.386 (3)	C27—C26	1.384 (3)
C7—H71	0.921	C27—H271	0.952
C6—C5	1.391 (3)	C26—C25	1.393 (2)
C6—H61	0.944	C26—H261	0.948
C5—C4	1.390 (2)	C25—C24	1.387 (2)
C5—H51	0.947	C25—H251	0.953
C4—H41	0.941	C24—H241	0.947
N1—N2	1.3845 (18)	N21—N22	1.3820 (18)
N1—H2	0.924	N21—H1	0.874
N2—C9	1.282 (2)	N22—C29	1.280 (2)
C9—C10	1.460 (2)	C29—C30	1.462 (2)
C9—H91	0.945	C29—H291	0.932
C10—C15	1.393 (2)	C30—C31	1.392 (2)
C10—C11	1.407 (2)	C30—C35	1.406 (2)
C15—C14	1.396 (2)	C31—C32	1.399 (2)
C15—H151	0.951	C31—H311	0.948
C14—C13	1.383 (2)	C32—C33	1.379 (2)
C14—H141	0.948	C32—H321	0.944
C13—O2	1.3612 (18)	C33—O21	1.3628 (18)
C13—C12	1.421 (2)	C33—C34	1.422 (2)
O2—C17	1.4325 (18)	O21—C36	1.4362 (18)
C17—H171	0.961	C36—H361	0.963
C17—H172	0.964	C36—H362	0.965
C17—H173	0.979	C36—H363	0.965
C12—C11	1.381 (2)	C34—C35	1.377 (2)
C12—O1	1.3603 (19)	C34—O22	1.3592 (19)
C11—H111	0.938	C35—H351	0.927
O1—C16	1.4273 (19)	O22—C37	1.4272 (18)
C16—H161	0.943	C37—H371	0.972
C16—H162	0.968	C37—H372	0.969
C16—H163	0.970	C37—H373	0.976
S1—C1—S2	125.49 (9)	S21—C21—S22	124.90 (9)
S1—C1—N1	120.52 (11)	S21—C21—N21	120.52 (11)
S2—C1—N1	113.98 (11)	S22—C21—N21	114.57 (11)

C1—S2—C2	102.05 (7)	C21—S22—C22	101.97 (7)
S2—C2—C3	107.65 (10)	S22—C22—C23	107.26 (10)
S2—C2—H21	110.3	S22—C22—H221	109.5
C3—C2—H21	109.7	C23—C22—H221	112.0
S2—C2—H22	107.9	S22—C22—H222	109.4
C3—C2—H22	110.5	C23—C22—H222	109.2
H21—C2—H22	110.7	H221—C22—H222	109.4
C2—C3—C8	121.01 (15)	C22—C23—C28	121.20 (14)
C2—C3—C4	119.67 (15)	C22—C23—C24	119.74 (15)
C8—C3—C4	119.32 (15)	C28—C23—C24	119.05 (14)
C3—C8—C7	120.44 (16)	C23—C28—C27	120.27 (15)
C3—C8—H81	119.0	C23—C28—H281	119.7
C7—C8—H81	120.5	C27—C28—H281	120.1
C8—C7—C6	120.09 (16)	C28—C27—C26	120.38 (16)
C8—C7—H71	120.5	C28—C27—H271	119.6
C6—C7—H71	119.5	C26—C27—H271	120.0
C7—C6—C5	119.73 (15)	C27—C26—C25	119.76 (15)
C7—C6—H61	118.7	C27—C26—H261	119.1
C5—C6—H61	121.5	C25—C26—H261	121.2
C6—C5—C4	120.34 (16)	C26—C25—C24	120.09 (16)
C6—C5—H51	119.1	C26—C25—H251	120.4
C4—C5—H51	120.6	C24—C25—H251	119.5
C3—C4—C5	120.06 (16)	C23—C24—C25	120.44 (16)
C3—C4—H41	118.9	C23—C24—H241	119.1
C5—C4—H41	121.1	C25—C24—H241	120.4
C1—N1—N2	120.71 (13)	C21—N21—N22	120.85 (12)
C1—N1—H2	118.7	C21—N21—H1	116.4
N2—N1—H2	120.6	N22—N21—H1	121.9
N1—N2—C9	113.83 (13)	N21—N22—C29	114.27 (13)
N2—C9—C10	122.28 (14)	N22—C29—C30	121.69 (14)
N2—C9—H91	120.4	N22—C29—H291	120.7
C10—C9—H91	117.3	C30—C29—H291	117.6
C9—C10—C15	117.98 (14)	C29—C30—C31	119.12 (14)
C9—C10—C11	122.42 (14)	C29—C30—C35	121.40 (14)
C15—C10—C11	119.58 (14)	C31—C30—C35	119.45 (14)
C10—C15—C14	120.50 (14)	C30—C31—C32	120.54 (14)
C10—C15—H151	120.0	C30—C31—H311	119.1
C14—C15—H151	119.5	C32—C31—H311	120.4
C15—C14—C13	120.08 (14)	C31—C32—C33	120.09 (14)
C15—C14—H141	119.4	C31—C32—H321	118.2
C13—C14—H141	120.5	C33—C32—H321	121.7
C14—C13—O2	125.39 (14)	C32—C33—O21	125.73 (13)
C14—C13—C12	119.77 (14)	C32—C33—C34	119.65 (14)
O2—C13—C12	114.83 (13)	O21—C33—C34	114.59 (13)
C13—O2—C17	117.10 (12)	C33—O21—C36	117.04 (12)
O2—C17—H171	106.1	O21—C36—H361	105.8
O2—C17—H172	111.9	O21—C36—H362	108.9
H171—C17—H172	109.6	H361—C36—H362	109.9

O2—C17—H173	109.3	O21—C36—H363	110.1
H171—C17—H173	109.9	H361—C36—H363	110.9
H172—C17—H173	110.0	H362—C36—H363	111.1
C13—C12—C11	119.89 (14)	C33—C34—C35	120.06 (14)
C13—C12—O1	114.08 (14)	C33—C34—O22	114.49 (13)
C11—C12—O1	126.01 (14)	C35—C34—O22	125.43 (14)
C10—C11—C12	120.16 (14)	C30—C35—C34	120.20 (14)
C10—C11—H111	120.7	C30—C35—H351	119.0
C12—C11—H111	119.1	C34—C35—H351	120.8
C12—O1—C16	117.16 (12)	C34—O22—C37	116.40 (12)
O1—C16—H161	106.2	O22—C37—H371	104.2
O1—C16—H162	110.2	O22—C37—H372	110.0
H161—C16—H162	111.1	H371—C37—H372	111.9
O1—C16—H163	110.8	O22—C37—H373	109.3
H161—C16—H163	110.4	H371—C37—H373	112.0
H162—C16—H163	108.1	H372—C37—H373	109.2

Hydrogen-bond geometry (Å, º)

Cg1, Cg2 and Cg4 are the centroids of the C3–C8, C10–C15 and C30–C35 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H2···S21	0.92	2.52	3.418 (1)	166
N21—H1···S1	0.87	2.55	3.407 (1)	168
C16—H163···O21^{i}	0.97	2.69	3.560 (2)	149
C17—H172···*Cg*4^{ii}	0.97	2.74	3.5587 (18)	143
C28—H281···*Cg*1^{ii}	0.94	2.94	3.6082 (18)	130
C36—H363···*Cg*2^{i}	0.97	2.67	3.5023 (17)	145

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