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Crystal structure of 2-(2,5-dimethoxyphenyl)-benzo[*d*]thiazole

Nadia H. Metwally,^a Galal H. Elgemeie^b and Peter G. Jones^{c*}^aChemistry Department, Faculty of Science, Cairo University, Giza, Egypt, ^bChemistry Department, Faculty of Science, Helwan University, Cairo, Egypt, and ^cInstitut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Hagenring 30, D-38106 Braunschweig, Germany. *Correspondence e-mail: p.jones@tu-bs.de

The title compound, C₁₅H₁₃NO₂S, was synthesized efficiently in the solid state by exploiting pepsin catalysis. The ring systems are nearly coplanar [interplanar angle of 5.38 (2)°] with an associated intramolecular S···O=C short contact of 2.7082 (4) Å. The packing involves C—H···O, C—H···π and π–π contacts.

1. Chemical context

Although countless synthetic methods are widely available, new and more efficient procedures or approaches are always needed. Enzymes, as ‘green’ catalysts for modern organic synthesis, have attracted increased attention because they may provide alternative and sustainable processes, thus helping to minimize the release of hazardous substances into the environment (Witayakran & Ragauskas, 2009). Pepsin, a kind of hydrolase, belongs to the family of aspartic acid proteases and is involved in chemical digestion of protein (Cooper *et al.*, 1990; Lin *et al.*, 1989). Pepsin-catalysed aldol (and other) reactions have been developed (Li *et al.*, 2010; He *et al.*, 2016; Zongbo *et al.*, 2017).

2-Aryl-benzothiazoles are a class of nitrogen-containing heterocyclic compounds that can be found in a variety of natural and synthetic compounds. In view of their biological and pharmacological characteristics, we are interested in developing synthetic strategies for heterocyclic ring systems containing a benzothiazole moiety; these have shown significant biological activity as novel antiviral and antimicrobial agents. (Azzam *et al.* 2017*a,b*, 2020*a,b,c*, 2021; Elgemeie *et al.*, 2000*a,b*, 2020). The conventional synthesis of 2-aryl-benzothiazoles, which involves heating a mixture containing 2-aminothiophenol (**1**), is disadvantageous because **1** is extremely unstable in air and highly toxic. In a continuation of our recent research in developing ‘green’ and simple syntheses of novel heterocyclic compounds (Metwally *et al.*, 2020, 2021*a,b*), we have now synthesized 2-(2,5-dimethoxyphenyl)benzo[*d*]thiazole (**3**) using pepsin as the ‘green’ catalytic reaction. Thus, a mixture of **1** and 2,5-dimethoxybenzaldehyde **2** was ground in a mortar with 0.05 g pepsin for 10 minutes, providing the desired product **3** in 97% yield. The nature of compound **3** was confirmed by spectroscopic analysis and by the single-crystal X-ray structure reported here.

2. Structural commentary

The structure of **3** is shown in Fig. 1. Molecular dimensions may be regarded as normal; a brief selection is presented in

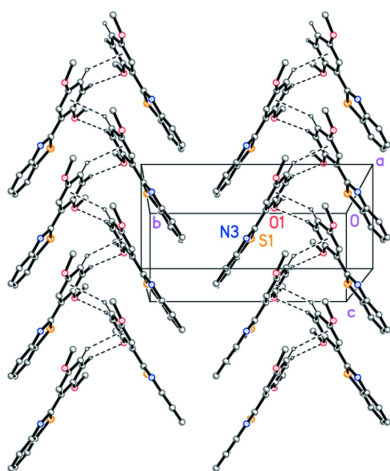
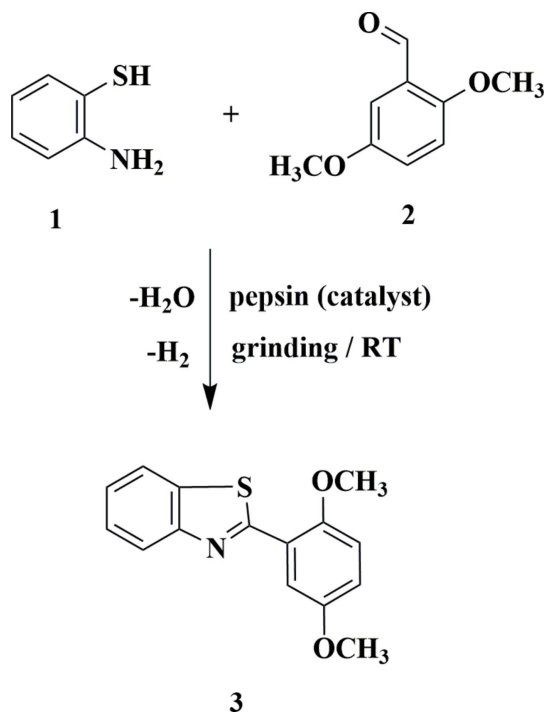


Table 1. Both ring systems are effectively planar (r.m.s. values of 0.01 Å for the benzothiazole and 0.004 Å for the phenyl ring, respectively), with an interplanar angle of 5.38 (2)°. The approximate coplanarity leads to the short intramolecular contacts S1···O1 = 2.7082 (4) and H16···N3 = 2.48 Å; the C16—H16···N3 angle is 101°.



3. Supramolecular features

There are no markedly short intermolecular contacts. One borderline ‘weak’ C—H···O hydrogen bond can be identified (Table 2), which links molecules *via* the *c*-glide operator $x, -y + \frac{1}{2}, z - \frac{1}{2}$. This is reinforced by a C—H··· π contact from H14 to the centroid of the phenyl ring (H14···Cg = 2.67 Å, C14—H14···Cg = 138°; Cg is the centroid of the C11—C16 ring). Additionally, the molecules are linked in pairs, related

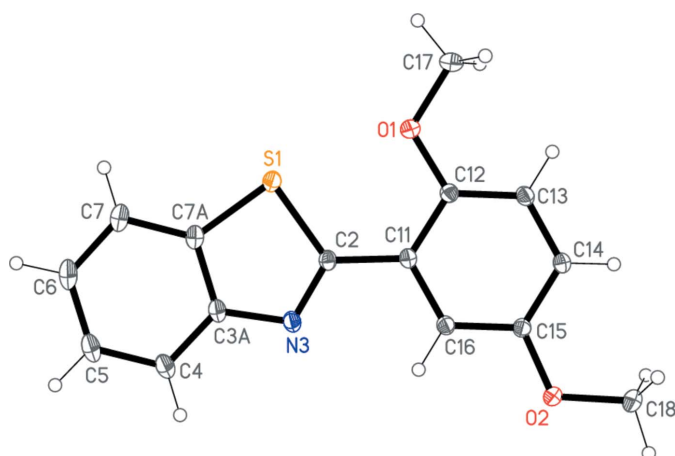


Figure 1
The molecule of **3** in the crystal. Ellipsoids represent 50% probability levels.

Table 1
Selected geometric parameters (Å, °).

S1—C7A	1.7327 (6)	N3—C3A	1.3820 (7)
S1—C2	1.7642 (5)	C3A—C7A	1.4082 (8)
C2—N3	1.3064 (7)		
C7A—S1—C2	89.40 (3)	N3—C3A—C7A	115.25 (5)
N3—C2—S1	114.72 (4)	C3A—C7A—S1	109.23 (4)
C2—N3—C3A	111.39 (5)		

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C13—H13···O1 ⁱ	0.95	2.65	3.5113 (7)	151
C18—H18C···N3 ⁱⁱ	0.98	2.60	3.4867 (8)	151

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

by *c*-axis translation, in which the benzothiazole ring system of one molecule lies opposite the phenyl ring of the other; the intercentroid distances are 3.5651 (3) Å for benzo···phenyl, and 3.6022 (3) Å for thiazole···phenyl (phenyl operator $x, y, -1 + z$). The net effect is to form a somewhat flattened herringbone pattern parallel to the *c* axis (Fig. 2; the π – π interactions are not shown explicitly). The contact C18—H18C···N3 (Table 2), involving a methyl group, connects the chains in the third dimension *via* the operator $-x + 1, -y + 1, -z$.

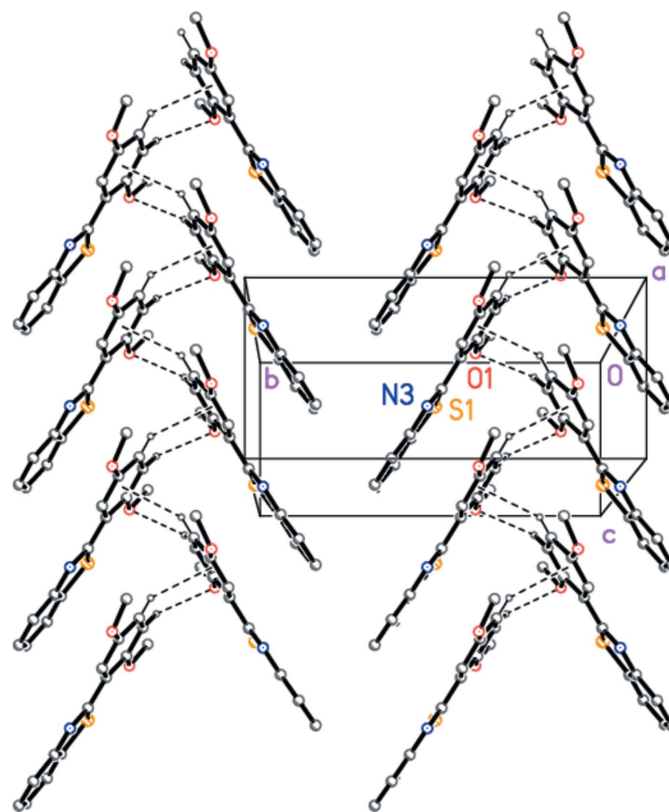


Figure 2
Crystal packing of **3**, viewed perpendicular to (100) in the region $x \approx 0.25$. Dashed lines indicate ‘weak’ C—H···O hydrogen bonds or C—H··· π contacts. Atom labels correspond to the asymmetric unit.

Table 3
Experimental details.

Crystal data	
Chemical formula	C ₁₅ H ₁₃ NO ₂ S
<i>M_r</i>	271.32
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.6666 (2), 13.8922 (2), 6.26063 (10)
β (°)	100.1273 (14)
<i>V</i> (Å ³)	1255.74 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.25
Crystal size (mm)	0.22 × 0.22 × 0.15
Data collection	
Diffraction	XtaLAB Synergy, HyPix
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2021)
<i>T_{min}</i> , <i>T_{max}</i>	0.927, 1.000
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	123768, 6759, 6156
<i>R_{int}</i>	0.023
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.871
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.027, 0.084, 1.04
No. of reflections	6759
No. of parameters	174
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.62, -0.19

Computer programs: *CrysAlis PRO* (Rigaku OD, 2021), *SHELXT* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *XP* (Siemens, 1994).

4. Database survey

A search of the Cambridge Database (Version 2021.3.0; Groom *et al.*, 2016) gave four hits for purely organic, neutral species in which one benzo[*d*]thiazole is bonded at its 2-position to an aromatic C₆ ring with oxygen substituents at the *ortho* (2-) and *meta* (5-) positions. These were CEFWOB [Yousuf *et al.*, 2012; 2-hydroxy, 5-methoxy; no S⋯O contact because of an intramolecular O–H⋯N hydrogen bond; interplanar angle 1.23 (9)°]; NOYSOM [Wang *et al.*, 2019; 2,5-dimethoxy with an additional 4-(2-pyridyl) substituent; two independent molecules; S⋯O = 2.650, 2.715 Å; interplanar angles of 6.0, 5.5°]; UFAHUF [Chen, 2007; 2,4,5-trimethoxy; S⋯O = 2.671 Å, interplanar angle of 4.5 (2)°] and WACPUO (Sakai *et al.*, 2016; 2-hydroxy, 5-methoxy with an additional 3-imidazole substituent; S⋯O = 2.695 Å, interplanar angle of 1.6°). Where not given in the original publications, these values were calculated using the CCDC program *Mercury* (Macrae *et al.*, 2020).

5. Synthesis and crystallization

A mixture of *o*-aminothiophenol **1** (0.01 mol), 2,5-dimethoxybenzaldehyde **2** (0.01 mol) and pepsin (0.05 g) was ground together at room temperature for 10 min. The viscous mixture was poured onto ice–water; the solid that formed was filtered off and recrystallized from ethanol to give pale-yellow crystals of **3** in 97% yield, m.p. 414 K; IR (KBr, cm⁻¹): ν_{max} 1581

(C=N); ¹H NMR (DMSO-*d*₆): δ = 3.82 (*s*, 3H, OCH₃), 4.0 (*s*, 3H, OCH₃), 7.13–7.15 (*m*, 1H, Ar), 7.22 (*d*, 1H, *J* = 8.8 Hz, Ar), 7.41 (*t*, 1H, *J* = 7.6 Hz, Ar), 7.51 (*t*, 1H, *J* = 7.6 Hz, Ar), 7.96 (*s*, 1H, Ar), 8.07 (*dd*, 2H, *J* = 8.0 Hz, Ar), ¹³C NMR (DMSO-*d*₆): δ = 56.0, 57.0, 112.5, 114.7, 119.1, 122.1, 122.2, 122.9, 125.4, 126.7, 136.0, 151.9, 153.8, 154.4, 162.3; *m/z* = 271 (*M*⁺, 100%), 238 (61.4%), 185 (27.6%), 136 (79.0%); Analysis: calculated for C₁₅H₁₃NO₂S (271.33) C 66.40, H 4.83, N 5.16, S 11.82%; found C 66.58, H 4.65, N 5.39, S 11.68%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Methyl groups were refined as idealized rigid groups allowed to rotate but not tip (AFIX 137), with C–H = 0.98 Å, H–C–H = 109.5°. Other hydrogen atoms were included using a riding model starting from calculated positions (C–H_{aromatic} = 0.95 Å). The *U*(H) values were fixed at 1.5 or 1.2 × *U*_{eq} of the parent carbon atoms for methyl and aromatic hydrogens, respectively.

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Crystal structure of 2-(2,5-dimethoxyphenyl)benzo[d]thiazole

Nadia H. Metwally, Galal H. Elgemeie and Peter G. Jones

Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL2018/3* (Sheldrick, 2015b).

2-(2,5-Dimethoxyphenyl)benzo[d]thiazole

Crystal data

$C_{15}H_{13}NO_2S$

$M_r = 271.32$

Monoclinic, $P2_1/c$

$a = 14.6666$ (2) Å

$b = 13.8922$ (2) Å

$c = 6.26063$ (10) Å

$\beta = 100.1273$ (14)°

$V = 1255.74$ (3) Å³

$Z = 4$

$F(000) = 568$

$D_x = 1.435$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 88513 reflections

$\theta = 2.8$ – 38.4 °

$\mu = 0.25$ mm⁻¹

$T = 100$ K

Block, colourless

$0.22 \times 0.22 \times 0.15$ mm

Data collection

XtaLAB Synergy, HyPix
diffractometer

Radiation source: micro-focus sealed X-ray tube

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(*CrysAlisPro*; Rigaku OD, 2021)

$T_{\min} = 0.927$, $T_{\max} = 1.000$

123768 measured reflections

6759 independent reflections

6156 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 38.3$ °, $\theta_{\min} = 2.0$ °

$h = -24 \rightarrow 25$

$k = -23 \rightarrow 23$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.084$

$S = 1.03$

6759 reflections

174 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.2455P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.62$ e Å⁻³

$\Delta\rho_{\min} = -0.19$ 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.

Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane)
 $-0.2606 (0.0025) x + 11.3686 (0.0009) y - 3.5208 (0.0006) z = 4.3561 (0.0009)$

* $-0.0113 (0.0003) S1 + 0.0122 (0.0004) C2 + 0.0073 (0.0004) N3 - 0.0022 (0.0005) C3A - 0.0178 (0.0004) C4 + 0.0029 (0.0005) C5 + 0.0151 (0.0005) C6 - 0.0033 (0.0005) C7 - 0.0029 (0.0005) C7A$

Rms deviation of fitted atoms = 0.0101

$-1.6150 (0.0031) x + 11.4261 (0.0017) y - 3.3180 (0.0011) z = 4.1087 (0.0012)$

Angle to previous plane (with approximate esd) = 5.381 (0.023)

* $-0.0035 (0.0003) C11 + 0.0058 (0.0004) C12 - 0.0025 (0.0004) C13 - 0.0031 (0.0004) C14 + 0.0054 (0.0004) C15 - 0.0020 (0.0004) C16 - 0.0003 (0.0008) O1 + 0.0801 (0.0011) C17 + 0.0285 (0.0008) O2 + 0.1636 (0.0010) C18$

Rms deviation of fitted atoms = 0.0040

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.13465 (2)	0.49165 (2)	0.34350 (2)	0.01451 (4)
C2	0.24674 (4)	0.47726 (4)	0.28209 (8)	0.01188 (8)
N3	0.31247 (3)	0.52002 (3)	0.41668 (7)	0.01347 (7)
C3A	0.27752 (4)	0.56826 (4)	0.57771 (8)	0.01360 (8)
C4	0.33134 (4)	0.62033 (4)	0.74630 (9)	0.01695 (9)
H4	0.396755	0.623486	0.758537	0.020*
C5	0.28692 (5)	0.66707 (4)	0.89466 (9)	0.01963 (10)
H5	0.322334	0.703577	1.008219	0.024*
C6	0.19042 (5)	0.66133 (5)	0.87976 (10)	0.02095 (11)
H6	0.161650	0.694472	0.982862	0.025*
C7	0.13610 (5)	0.60805 (4)	0.71696 (10)	0.01924 (10)
H7	0.071002	0.603042	0.709129	0.023*
C7A	0.18087 (4)	0.56196 (4)	0.56475 (9)	0.01468 (8)
C11	0.26660 (3)	0.42388 (3)	0.09270 (8)	0.01131 (7)
C12	0.19879 (3)	0.37320 (4)	-0.05164 (8)	0.01179 (8)
C13	0.22303 (4)	0.32478 (4)	-0.22766 (8)	0.01295 (8)
H13	0.177114	0.290066	-0.323243	0.016*
C14	0.31402 (4)	0.32648 (4)	-0.26592 (8)	0.01283 (8)
H14	0.329903	0.293120	-0.386674	0.015*
C15	0.38132 (3)	0.37743 (4)	-0.12577 (8)	0.01215 (8)
C16	0.35765 (4)	0.42522 (4)	0.05254 (8)	0.01240 (8)
H16	0.404004	0.459248	0.148423	0.015*
O1	0.11061 (3)	0.37347 (3)	-0.00594 (7)	0.01587 (7)
C17	0.04056 (4)	0.32676 (5)	-0.15693 (10)	0.01998 (10)
H17A	0.036645	0.356648	-0.300050	0.030*
H17B	-0.019153	0.333071	-0.108453	0.030*
H17C	0.056005	0.258430	-0.166186	0.030*
O2	0.47191 (3)	0.38509 (3)	-0.15047 (7)	0.01691 (8)
C18	0.49545 (4)	0.34434 (5)	-0.34295 (10)	0.01952 (10)
H18A	0.454902	0.371139	-0.470203	0.029*

H18B	0.487554	0.274329	-0.340465	0.029*
H18C	0.560067	0.359596	-0.350301	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01415 (6)	0.01602 (6)	0.01373 (6)	0.00148 (4)	0.00352 (4)	-0.00175 (4)
C2	0.01436 (18)	0.01083 (17)	0.01076 (17)	0.00014 (14)	0.00307 (14)	0.00011 (13)
N3	0.01641 (18)	0.01302 (17)	0.01139 (16)	-0.00157 (13)	0.00354 (13)	-0.00175 (13)
C3A	0.0193 (2)	0.01086 (18)	0.01120 (17)	-0.00042 (15)	0.00426 (15)	-0.00038 (14)
C4	0.0236 (2)	0.0142 (2)	0.01336 (19)	-0.00312 (17)	0.00403 (17)	-0.00254 (15)
C5	0.0314 (3)	0.0140 (2)	0.0142 (2)	-0.00201 (19)	0.00606 (19)	-0.00317 (16)
C6	0.0321 (3)	0.0161 (2)	0.0167 (2)	0.0025 (2)	0.0097 (2)	-0.00306 (17)
C7	0.0239 (2)	0.0180 (2)	0.0176 (2)	0.00356 (19)	0.00846 (19)	-0.00219 (18)
C7A	0.0190 (2)	0.01267 (19)	0.01312 (18)	0.00175 (15)	0.00489 (15)	-0.00059 (15)
C11	0.01340 (17)	0.01037 (17)	0.01029 (16)	0.00010 (13)	0.00241 (13)	-0.00034 (13)
C12	0.01206 (17)	0.01134 (18)	0.01187 (17)	0.00064 (13)	0.00182 (14)	-0.00025 (13)
C13	0.01318 (18)	0.01267 (18)	0.01268 (18)	0.00015 (14)	0.00138 (14)	-0.00222 (14)
C14	0.01418 (18)	0.01223 (18)	0.01217 (18)	0.00012 (14)	0.00257 (14)	-0.00183 (14)
C15	0.01276 (18)	0.01177 (18)	0.01232 (17)	-0.00073 (14)	0.00333 (14)	-0.00073 (14)
C16	0.01365 (18)	0.01212 (18)	0.01161 (17)	-0.00128 (14)	0.00273 (14)	-0.00118 (14)
O1	0.01170 (15)	0.01927 (18)	0.01672 (16)	-0.00048 (12)	0.00270 (12)	-0.00411 (13)
C17	0.01240 (19)	0.0272 (3)	0.0192 (2)	-0.00078 (18)	-0.00011 (17)	-0.0035 (2)
O2	0.01379 (16)	0.02132 (19)	0.01681 (17)	-0.00358 (13)	0.00599 (13)	-0.00600 (14)
C18	0.0175 (2)	0.0238 (3)	0.0190 (2)	-0.00194 (19)	0.00813 (18)	-0.00580 (19)

Geometric parameters (Å, °)

S1—C7A	1.7327 (6)	C15—O2	1.3686 (6)
S1—C2	1.7642 (5)	C15—C16	1.3941 (7)
C2—N3	1.3064 (7)	O1—C17	1.4243 (7)
C2—C11	1.4704 (7)	O2—C18	1.4276 (7)
N3—C3A	1.3820 (7)	C4—H4	0.9500
C3A—C4	1.4027 (8)	C5—H5	0.9500
C3A—C7A	1.4082 (8)	C6—H6	0.9500
C4—C5	1.3862 (8)	C7—H7	0.9500
C5—C6	1.4043 (10)	C13—H13	0.9500
C6—C7	1.3912 (9)	C14—H14	0.9500
C7—C7A	1.4032 (8)	C16—H16	0.9500
C11—C16	1.4017 (7)	C17—H17A	0.9800
C11—C12	1.4091 (7)	C17—H17B	0.9800
C12—O1	1.3728 (6)	C17—H17C	0.9800
C12—C13	1.3896 (7)	C18—H18A	0.9800
C13—C14	1.3969 (7)	C18—H18B	0.9800
C14—C15	1.3930 (7)	C18—H18C	0.9800
C7A—S1—C2	89.40 (3)	C15—O2—C18	116.63 (4)
N3—C2—C11	121.40 (5)	C5—C4—H4	120.7

N3—C2—S1	114.72 (4)	C3A—C4—H4	120.7
C11—C2—S1	123.86 (4)	C4—C5—H5	119.5
C2—N3—C3A	111.39 (5)	C6—C5—H5	119.5
N3—C3A—C4	124.55 (5)	C7—C6—H6	119.4
N3—C3A—C7A	115.25 (5)	C5—C6—H6	119.4
C4—C3A—C7A	120.20 (5)	C6—C7—H7	121.2
C5—C4—C3A	118.50 (6)	C7A—C7—H7	121.2
C4—C5—C6	121.05 (6)	C12—C13—H13	119.6
C7—C6—C5	121.30 (5)	C14—C13—H13	119.6
C6—C7—C7A	117.66 (6)	C15—C14—H14	120.2
C7—C7A—C3A	121.26 (5)	C13—C14—H14	120.2
C7—C7A—S1	129.51 (5)	C15—C16—H16	119.5
C3A—C7A—S1	109.23 (4)	C11—C16—H16	119.5
C16—C11—C12	118.61 (4)	O1—C17—H17A	109.5
C16—C11—C2	117.91 (4)	O1—C17—H17B	109.5
C12—C11—C2	123.47 (4)	H17A—C17—H17B	109.5
O1—C12—C13	123.26 (5)	O1—C17—H17C	109.5
O1—C12—C11	116.71 (4)	H17A—C17—H17C	109.5
C13—C12—C11	120.02 (5)	H17B—C17—H17C	109.5
C12—C13—C14	120.88 (5)	O2—C18—H18A	109.5
C15—C14—C13	119.54 (5)	O2—C18—H18B	109.5
O2—C15—C14	124.24 (5)	H18A—C18—H18B	109.5
O2—C15—C16	115.90 (4)	O2—C18—H18C	109.5
C14—C15—C16	119.85 (5)	H18A—C18—H18C	109.5
C15—C16—C11	121.10 (5)	H18B—C18—H18C	109.5
C12—O1—C17	117.16 (4)		
C7A—S1—C2—N3	0.85 (4)	S1—C2—C11—C16	174.46 (4)
C7A—S1—C2—C11	-177.67 (4)	N3—C2—C11—C12	177.18 (5)
C11—C2—N3—C3A	177.97 (4)	S1—C2—C11—C12	-4.38 (7)
S1—C2—N3—C3A	-0.60 (6)	C16—C11—C12—O1	179.80 (5)
C2—N3—C3A—C4	179.57 (5)	C2—C11—C12—O1	-1.36 (7)
C2—N3—C3A—C7A	-0.08 (7)	C16—C11—C12—C13	0.89 (7)
N3—C3A—C4—C5	178.64 (5)	C2—C11—C12—C13	179.73 (5)
C7A—C3A—C4—C5	-1.73 (8)	O1—C12—C13—C14	-179.65 (5)
C3A—C4—C5—C6	1.12 (9)	C11—C12—C13—C14	-0.81 (8)
C4—C5—C6—C7	0.50 (10)	C12—C13—C14—C15	-0.03 (8)
C5—C6—C7—C7A	-1.46 (9)	C13—C14—C15—O2	-178.84 (5)
C6—C7—C7A—C3A	0.83 (9)	C13—C14—C15—C16	0.78 (8)
C6—C7—C7A—S1	-179.51 (5)	O2—C15—C16—C11	178.96 (5)
N3—C3A—C7A—C7	-179.57 (5)	C14—C15—C16—C11	-0.69 (8)
C4—C3A—C7A—C7	0.76 (8)	C12—C11—C16—C15	-0.14 (7)
N3—C3A—C7A—S1	0.70 (6)	C2—C11—C16—C15	-179.05 (5)
C4—C3A—C7A—S1	-178.96 (4)	C13—C12—O1—C17	-4.35 (8)
C2—S1—C7A—C7	179.48 (6)	C11—C12—O1—C17	176.78 (5)
C2—S1—C7A—C3A	-0.82 (4)	C14—C15—O2—C18	5.35 (8)
N3—C2—C11—C16	-3.97 (7)	C16—C15—O2—C18	-174.28 (5)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C13—H13···O1 ⁱ	0.95	2.65	3.5113 (7)	151
C18—H18C···N3 ⁱⁱ	0.98	2.60	3.4867 (8)	151

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