

# Benzyl 2-(benzylsulfanyl)benzoate

Zorica Leka,<sup>a\*</sup> Sladjana B. Novaković,<sup>b</sup> Goran A. Bogdanović,<sup>b</sup> Gordana P. Radić<sup>c</sup> and Zoran R. Ratković<sup>d</sup>

<sup>a</sup>Faculty of Metallurgy and Technology, University of Montenegro, Cetinjski put bb, 81000 Podgorica, Montenegro, <sup>b</sup>Vinča Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, University of Belgrade, PO Box 522, 11001 Belgrade, Serbia, <sup>c</sup>Faculty of Medical Sciences, University of Kragujevac, S. Markovića 69, 34000 Kragujevac, Serbia, and <sup>d</sup>Department of Chemistry, Faculty of Science, University of Kragujevac, R. Domanovića 12, 34000 Kragujevac, Serbia  
Correspondence e-mail: zorica@ac.me

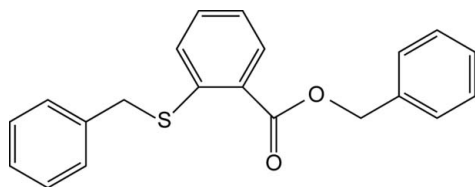
Received 9 January 2013; accepted 17 January 2013

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.040;  $wR$  factor = 0.113; data-to-parameter ratio = 15.2.

In the title compound,  $\text{C}_{21}\text{H}_{18}\text{O}_2\text{S}$ , the central aromatic ring makes dihedral angles of  $5.86$  (12) and  $72.02$  (6)° with the rings of the terminal *O*-benzyl and *S*-benzyl groups, respectively. The dihedral angle between the peripheral phenyl rings is  $66.16$  (6)°. In the crystal, molecules are linked by pairs of  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds, forming inversion dimers. These dimers are linked *via*  $\text{C}-\text{H}\cdots\pi$  interactions, forming a three-dimensional network.

## Related literature

For related structures, see: Radić *et al.* (2012); Lucena *et al.* (1996); Sillanpää *et al.* (1994); Alhadi *et al.* (2010). For the biological activity of thiosalicylic acid derivatives, see: Bernardelli *et al.* (2005); Halaschek-Wiener *et al.* (2003); Sadao *et al.* (2000).



## Experimental

### Crystal data

$\text{C}_{21}\text{H}_{18}\text{O}_2\text{S}$   
 $M_r = 334.41$   
 Triclinic,  $P\bar{1}$   
 $a = 5.6957$  (3) Å  
 $b = 12.1117$  (11) Å  
 $c = 13.0813$  (11) Å  
 $\alpha = 72.748$  (8)°  
 $\beta = 86.477$  (6)°  
 $\gamma = 89.941$  (6)°  
 $V = 860.04$  (12) Å<sup>3</sup>  
 $Z = 2$   
 Cu  $K\alpha$  radiation  
 $\mu = 1.74$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.11 \times 0.10 \times 0.05$  mm

### Data collection

Oxford Diffraction Xcalibur Gemini Sapphire3 diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2012)  
 $T_{\min} = 0.944$ ,  $T_{\max} = 1.000$   
 5368 measured reflections  
 3299 independent reflections  
 2554 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.113$   
 $S = 1.04$   
 3299 reflections  
 217 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.21$  e Å<sup>-3</sup>

**Table 1**

Geometry of hydrogen bonds and weak  $\text{C}-\text{H}\cdots\pi$  interactions (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C2–C7, C9–C14 and C16–C21 rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
C14–H14 $\cdots$ O2 <sup>i</sup>	0.93	2.63	3.408 (3)	142
C4–H4 $\cdots$ Cg3 <sup>ii</sup>	0.93	3.11	3.846 (3)	137
C13–H13 $\cdots$ Cg3 <sup>i</sup>	0.93	2.88	3.653 (3)	141
C18–H18 $\cdots$ Cg1 <sup>iii</sup>	0.93	3.20	3.820 (3)	126
C20–H20 $\cdots$ Cg2 <sup>iv</sup>	0.93	2.96	3.651 (3)	132

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009) and *PARST* (Nardelli, 1995).

This work was supported by the Ministry of Education and Science of the Republic of Serbia (Project Nos. 172016, 172034, 172014 and 172035). We thank Professor V. Divjakovic, University of Novi Sad, for help with the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ5036).

## References

- Alhadi, A. A., Khaledi, H., Mohd Ali, H. & Olmstead, M. M. (2010). *Acta Cryst.* **E66**, o1787.  
 Bernardelli, P., Cronin, A. M., Denis, A., Denton, S. M., Jacobelli, H., Kemp, M. I., Lorthiois, E., Rousseau, F., Serradeil-Civit, D. & Vergne, F. (2005). US Patent 20050267095.  
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.  
 Halaschek-Wiener, J., Kloog, Y., Wacheck, V. & Jansen, B. (2003). *J. Invest. Dermatol.* **120**, 109–115.  
 Lucena, N., Casabó, J., Escriche, L., Sánchez-Castelló, G., Teixidor, F., Kivekäs, R. & Sillanpää, R. (1996). *Polyhedron*, **15**, 3009–3018.  
 Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.  
 Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.  
 Oxford Diffraction (2012). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.

- Radić, G. P., Glodjović, V. V., Radojević, I. D., Stefanović, O. D., Čomić, Lj. R., Ratković, Z. R., Valkonen, A., Rissanen, K. & Trifunović, S. R. (2012). *Polyhedron*, **31**, 69–76.
- Sadao, I., Fujio, S., Hidekazu, M. & Keita, K. (2000). Jpn Patent 2000-178188.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sillanpää, R., Kivekäs, R., Escriche, L., Lucena, N., Teixidor, F. & Casabó, J. (1994). *Acta Cryst.* **C50**, 2049–2051.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

## supporting information

*Acta Cryst.* (2013). E69, o285–o286 [doi:10.1107/S1600536813001761]

**Benzyl 2-(benzylsulfanyl)benzoate**

**Zorica Leka, Sladjana B. Novaković, Goran A. Bogdanović, Gordana P. Radić and Zoran R. Ratković**

**S1. Comment**

Thiosalicylic acid and its derivatives find potential application in numerous disease treatments, in particular inflammatory, allergic and respiratory diseases (Bernardelli *et al.*, 2005) as well as Ras tumor growth inhibitors (Halaschek-Wiener *et al.*, 2003). Ketones derived from thiosalicylic acids have application as bile acid transport inhibitors (Sadao *et al.*, 2000). In continuation of our work on structural and biological properties of thiosalicylic derivatives and their metal complexes (Radić *et al.*, 2012) here we present the crystal structure of the novel ligand benzyl 2-(benzylsulfanyl)benzoate.

The bond lengths and angles in the title compound are within the expected ranges. The dihedral angle between aromatic rings of the central thiosalicylic and terminal *O*-benzyl group is 5.86 (12)° indicating a nearly co-planar orientation of these two fragments. On the other hand, the ring of the *S*-benzyl group is significantly twisted with respect to the central ring forming a dihedral angle of 72.02 (6)°. In the previously reported crystal structures with *S*-benzyl derivatives of thiosalicylic acid the analogue dihedral angle varies from 13.4 to 88.9°, suggesting the free rotation of the *S*-benzyl ring around the single bonds of the C3–S1–C15–C16 fragment. The specific property of the present compound is that the atoms S1, C15 and C16 all lie in the plane of the central ring within 0.03 Å. In the cases of similar uncoordinated (Sillanpää *et al.*, 1994; Alhadi *et al.*, 2010] as well as coordinated ligands (Radić *et al.*, 2012; Lucena *et al.*, 1996) the corresponding atom C16 is significantly out of the central ring plane (1.57 Å in average).

The pair of C14—H14⋯O2 interactions connects inversion related molecules into dimers (Table 1, Fig. 2). This connection is reinforced by means of C—H⋯ $\pi$  interactions involving the *O*-benzyl C13—H13 donor and the *S*-benzyl ring from an inversion-related molecule as acceptor (Table 1; Cg3 is the centroid of the *S*-benzyl ring). The *S*-benzyl ring also serves as a  $\pi$ -acceptor for C—H donors of a neighboring molecular pair; in that way the pairs of molecules further arrange into chain by C4—H4⋯Cg3 interactions (Table 1, Fig. 2). The molecules are further associated into a three-dimensional structure by C—H⋯ $\pi$  interactions which engage two remaining phenyl rings as  $\pi$ -acceptors (Table 1, Cg1 and Cg2 are centroids of central thiosalicylic and terminal *O*-benzyl rings, respectively).

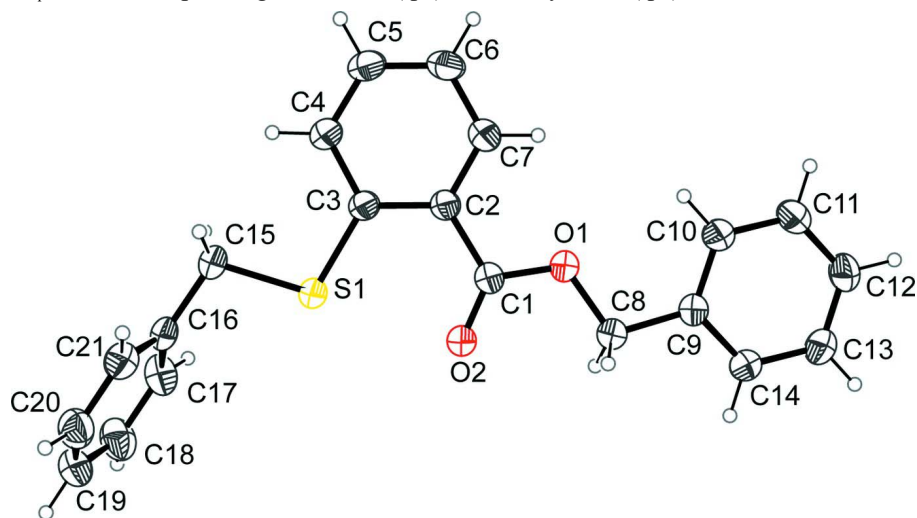
**S2. Experimental**

The thioacid ligand was prepared by alkylation of thiosalicylic acid by means of the corresponding alkyl halogenides in alkaline water-ethanol solution. Thiosalicylic acid (1 mmol) was added to a 100 cm<sup>3</sup> round bottom flask containing 50 cm<sup>3</sup> of a 30% solution of ethanol in water and stirred. A solution of NaOH (2 mmol in 5 cm<sup>3</sup> of water) was added to the acid suspension, whereupon the solution became clear. The corresponding benzyl halogenide (2 mmol) was dissolved in 5 cm<sup>3</sup> of ethanol and transferred to the stirred solution. The resulting mixture was kept overnight at 60°C. The reaction mixture was transferred into a beaker and ethanol was evaporated off on a water bath. Diluted hydrochloric acid (2 mol/dm<sup>3</sup>) was added to the resulting water solution and *S*-benzyl thiosalicylic acid was precipitated as a white powder.

The obtained acid was filtered off and washed with plenty of distilled water. The product was dried under vacuum overnight. Crystals of the title compound suitable for X-ray determination were obtained by slow evaporation of a benzyl alcohol solution, which unexpectedly resulted in the esterification of the carboxylic group of thiosalicylic acid.

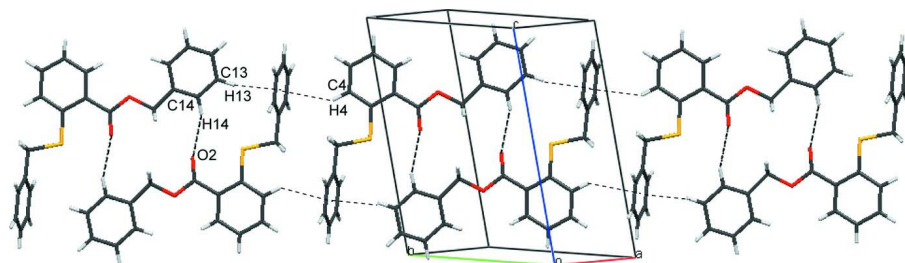
### S3. Refinement

H atoms bonded to C atoms were placed at geometrically calculated positions and refined using a riding model. C—H distances were fixed to 0.93 and 0.97 Å from aromatic and methylene C atoms, respectively. The  $U_{\text{iso}}(\text{H})$  values were equal to 1.2 times  $U_{\text{eq}}$  of the corresponding aromatic  $\text{C}(sp^2)$  and methylene  $\text{C}(sp^3)$  atoms.



**Figure 1**

The molecular structure of the title compound with 40% probability displacement ellipsoids for non-H atoms.



**Figure 2**

Partial crystal packing of the title compound. The C14—H $\cdots$ O2 and C13—H $\cdots$  $\pi$  connected pairs of molecules are linked into a chain by C4—H4 $\cdots$  $\pi$  interactions.

### Benzyl 2-(benzylsulfanyl)benzoate

#### Crystal data

$\text{C}_{21}\text{H}_{18}\text{O}_2\text{S}$

$M_r = 334.41$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 5.6957(3)\ \text{\AA}$

$b = 12.1117(11)\ \text{\AA}$

$c = 13.0813(11)\ \text{\AA}$

$\alpha = 72.748(8)^\circ$

$\beta = 86.477(6)^\circ$

$\gamma = 89.941(6)^\circ$

$V = 860.04(12)\ \text{\AA}^3$

$Z = 2$

$F(000) = 352$

$D_x = 1.291\ \text{Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.54180\ \text{\AA}$

Cell parameters from 2123 reflections

$\theta = 3.5\text{--}72.3^\circ$   
 $\mu = 1.74 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$

Prism, colourless  
 $0.11 \times 0.10 \times 0.05 \text{ mm}$

*Data collection*

Oxford Diffraction Xcalibur Gemini Sapphire3 diffractometer  
 Radiation source: Enhance (Cu) X-ray Source Graphite monochromator  
 Detector resolution:  $16.3280 \text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan (CrysAlis PRO; Oxford Diffraction, 2012)  
 $T_{\min} = 0.944, T_{\max} = 1.000$

5368 measured reflections  
 3299 independent reflections  
 2554 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$   
 $\theta_{\max} = 72.4^\circ, \theta_{\min} = 3.6^\circ$   
 $h = -5 \rightarrow 7$   
 $k = -14 \rightarrow 14$   
 $l = -16 \rightarrow 15$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.113$   
 $S = 1.04$   
 3299 reflections  
 217 parameters  
 0 restraints  
 Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map  
 Hydrogen site location: inferred from neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.0651P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{Å}^{-3}$

*Special details*

**Experimental.** IR (KBr,  $\text{cm}^{-1}$ ): 3414, 3061, 2920, 2648, 2559, 1674, 1584, 1562, 1463, 1412, 1317, 1272, 1255, 1154, 1062, 1046, 897, 743, 711, 652, 551.  $^1\text{H}$  NMR (200 MHz,  $\text{CDCl}_3$ ,  $\delta$  p.p.m.): 4.11 (s, 2H,  $\text{C}^{15}\text{H}_2$ ), 5.45 (s, 2H,  $\text{C}^8\text{H}_2$ ), 7.00–7.93 (m, 17H, Ar and bz).  $^{13}\text{C}$  NMR (50 MHz,  $\text{DMSO-d}_6$ ,  $\delta$  p.p.m.): 38.5 ( $\text{C}^{15}\text{H}_2$ ), 68.3 ( $\text{C}^8\text{H}_2$ ), 125.0; 126.3; 126.8; 127.0; 127.2; 127.5; 127.8; 127.9; 128.1; 128.3; 128.8; 128.9; 129.3; 130.2; 133.5; 139.5; 141.7; 142.3 (Ar and bz), 166.8 (COObz).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{Å}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.60616 (9)	0.22258 (5)	0.48163 (4)	0.06178 (18)
O1	0.1278 (2)	0.47589 (12)	0.28903 (10)	0.0595 (4)
O2	0.2518 (3)	0.37675 (15)	0.44697 (11)	0.0859 (6)
C1	0.2696 (3)	0.40163 (17)	0.35128 (15)	0.0549 (5)
C2	0.4509 (3)	0.35644 (16)	0.28855 (14)	0.0519 (4)
C3	0.6149 (3)	0.27491 (16)	0.34054 (14)	0.0519 (4)
C4	0.7850 (4)	0.23806 (19)	0.27595 (16)	0.0632 (5)
H4	0.8945	0.1838	0.3081	0.076*
C5	0.7919 (4)	0.2808 (2)	0.16621 (17)	0.0728 (6)
H5	0.9072	0.2555	0.1253	0.087*
C6	0.6324 (4)	0.3601 (2)	0.11575 (17)	0.0743 (6)
H6	0.6388	0.3885	0.0413	0.089*
C7	0.4622 (4)	0.39694 (19)	0.17718 (15)	0.0650 (5)
H7	0.3525	0.4501	0.1433	0.078*
C8	-0.0440 (4)	0.53023 (19)	0.34328 (15)	0.0602 (5)

H8A	0.0348	0.5751	0.3817	0.072*
H8B	-0.1426	0.4718	0.3946	0.072*
C9	-0.1923 (3)	0.60777 (16)	0.26112 (15)	0.0522 (4)
C10	-0.1380 (4)	0.6363 (2)	0.15204 (16)	0.0659 (6)
H10	-0.0031	0.6073	0.1264	0.079*
C11	-0.2821 (4)	0.7076 (2)	0.08082 (17)	0.0725 (6)
H11	-0.2437	0.7260	0.0075	0.087*
C12	-0.4810 (4)	0.7514 (2)	0.11702 (18)	0.0712 (6)
H12	-0.5780	0.7990	0.0686	0.085*
C13	-0.5362 (4)	0.7247 (2)	0.22537 (18)	0.0678 (6)
H13	-0.6698	0.7552	0.2505	0.081*
C14	-0.3935 (3)	0.65252 (18)	0.29709 (16)	0.0592 (5)
H14	-0.4332	0.6339	0.3703	0.071*
C15	0.8417 (4)	0.11867 (19)	0.50644 (16)	0.0637 (5)
H15A	0.8106	0.0571	0.4754	0.076*
H15B	0.9904	0.1561	0.4746	0.076*
C16	0.8515 (3)	0.07081 (16)	0.62584 (15)	0.0555 (5)
C17	0.6840 (4)	-0.0071 (2)	0.68695 (18)	0.0715 (6)
H17	0.5632	-0.0315	0.6536	0.086*
C18	0.6927 (4)	-0.0493 (2)	0.79649 (19)	0.0817 (7)
H18	0.5787	-0.1022	0.8364	0.098*
C19	0.8689 (4)	-0.0138 (2)	0.84739 (19)	0.0757 (6)
H19	0.8743	-0.0418	0.9215	0.091*
C20	1.0364 (4)	0.0634 (2)	0.78757 (19)	0.0746 (6)
H20	1.1571	0.0872	0.8214	0.090*
C21	1.0283 (4)	0.10629 (19)	0.67754 (17)	0.0641 (5)
H21	1.1423	0.1594	0.6380	0.077*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0688 (3)	0.0641 (3)	0.0475 (3)	0.0269 (2)	-0.0004 (2)	-0.0098 (2)
O1	0.0647 (8)	0.0623 (8)	0.0502 (7)	0.0208 (7)	-0.0064 (6)	-0.0145 (6)
O2	0.0995 (12)	0.1023 (13)	0.0475 (8)	0.0567 (10)	-0.0012 (7)	-0.0103 (8)
C1	0.0607 (11)	0.0530 (11)	0.0481 (10)	0.0107 (9)	-0.0047 (8)	-0.0106 (8)
C2	0.0601 (11)	0.0465 (10)	0.0469 (10)	0.0058 (8)	0.0000 (8)	-0.0111 (8)
C3	0.0570 (11)	0.0489 (10)	0.0483 (10)	0.0060 (8)	0.0028 (8)	-0.0136 (8)
C4	0.0660 (12)	0.0638 (13)	0.0567 (11)	0.0154 (10)	0.0050 (9)	-0.0152 (9)
C5	0.0790 (15)	0.0769 (15)	0.0615 (13)	0.0124 (12)	0.0148 (10)	-0.0229 (11)
C6	0.0987 (17)	0.0748 (15)	0.0450 (11)	0.0102 (13)	0.0089 (11)	-0.0139 (10)
C7	0.0794 (14)	0.0618 (13)	0.0501 (11)	0.0136 (11)	-0.0039 (10)	-0.0109 (9)
C8	0.0645 (12)	0.0638 (12)	0.0502 (11)	0.0173 (10)	-0.0028 (9)	-0.0138 (9)
C9	0.0542 (10)	0.0489 (10)	0.0523 (10)	0.0059 (8)	-0.0050 (8)	-0.0129 (8)
C10	0.0618 (12)	0.0783 (15)	0.0537 (11)	0.0165 (11)	-0.0007 (9)	-0.0142 (10)
C11	0.0755 (14)	0.0837 (16)	0.0506 (11)	0.0134 (12)	-0.0052 (10)	-0.0077 (10)
C12	0.0655 (13)	0.0764 (15)	0.0673 (14)	0.0172 (11)	-0.0186 (10)	-0.0120 (11)
C13	0.0591 (12)	0.0716 (14)	0.0738 (14)	0.0181 (10)	-0.0061 (10)	-0.0228 (11)
C14	0.0609 (12)	0.0636 (12)	0.0546 (11)	0.0099 (10)	-0.0031 (9)	-0.0202 (9)

C15	0.0637 (12)	0.0635 (12)	0.0621 (12)	0.0257 (10)	-0.0048 (9)	-0.0160 (10)
C16	0.0553 (11)	0.0490 (10)	0.0615 (12)	0.0180 (9)	-0.0052 (9)	-0.0150 (9)
C17	0.0682 (13)	0.0626 (13)	0.0766 (15)	0.0004 (11)	-0.0176 (11)	-0.0073 (11)
C18	0.0813 (16)	0.0699 (15)	0.0762 (16)	-0.0043 (12)	-0.0062 (12)	0.0059 (12)
C19	0.0878 (17)	0.0730 (15)	0.0603 (13)	0.0167 (13)	-0.0134 (12)	-0.0091 (11)
C20	0.0734 (15)	0.0783 (16)	0.0769 (15)	0.0095 (12)	-0.0201 (12)	-0.0272 (13)
C21	0.0563 (12)	0.0637 (13)	0.0717 (14)	0.0039 (10)	-0.0022 (10)	-0.0197 (10)

*Geometric parameters (Å, °)*

S1—C3	1.7623 (19)	C10—H10	0.9300
S1—C15	1.8159 (18)	C11—C12	1.368 (3)
O1—C1	1.331 (2)	C11—H11	0.9300
O1—C8	1.444 (2)	C12—C13	1.373 (3)
O2—C1	1.195 (2)	C12—H12	0.9300
C1—C2	1.483 (3)	C13—C14	1.382 (3)
C2—C7	1.390 (2)	C13—H13	0.9300
C2—C3	1.410 (3)	C14—H14	0.9300
C3—C4	1.405 (2)	C15—C16	1.501 (3)
C4—C5	1.372 (3)	C15—H15A	0.9700
C4—H4	0.9300	C15—H15B	0.9700
C5—C6	1.371 (3)	C16—C17	1.379 (3)
C5—H5	0.9300	C16—C21	1.383 (3)
C6—C7	1.379 (3)	C17—C18	1.375 (3)
C6—H6	0.9300	C17—H17	0.9300
C7—H7	0.9300	C18—C19	1.375 (3)
C8—C9	1.504 (2)	C18—H18	0.9300
C8—H8A	0.9700	C19—C20	1.368 (3)
C8—H8B	0.9700	C19—H19	0.9300
C9—C10	1.380 (3)	C20—C21	1.381 (3)
C9—C14	1.383 (3)	C20—H20	0.9300
C10—C11	1.379 (3)	C21—H21	0.9300
C3—S1—C15	103.19 (9)	C12—C11—H11	119.7
C1—O1—C8	116.17 (14)	C10—C11—H11	119.7
O2—C1—O1	122.68 (18)	C11—C12—C13	119.5 (2)
O2—C1—C2	124.83 (17)	C11—C12—H12	120.2
O1—C1—C2	112.48 (16)	C13—C12—H12	120.2
C7—C2—C3	119.66 (17)	C12—C13—C14	120.1 (2)
C7—C2—C1	119.51 (17)	C12—C13—H13	120.0
C3—C2—C1	120.82 (16)	C14—C13—H13	120.0
C4—C3—C2	117.65 (17)	C13—C14—C9	120.71 (19)
C4—C3—S1	121.64 (15)	C13—C14—H14	119.6
C2—C3—S1	120.71 (14)	C9—C14—H14	119.6
C5—C4—C3	121.03 (19)	C16—C15—S1	107.11 (13)
C5—C4—H4	119.5	C16—C15—H15A	110.3
C3—C4—H4	119.5	S1—C15—H15A	110.3
C6—C5—C4	121.3 (2)	C16—C15—H15B	110.3

C6—C5—H5	119.4	S1—C15—H15B	110.3
C4—C5—H5	119.4	H15A—C15—H15B	108.5
C5—C6—C7	118.9 (2)	C17—C16—C21	118.3 (2)
C5—C6—H6	120.5	C17—C16—C15	121.5 (2)
C7—C6—H6	120.5	C21—C16—C15	120.2 (2)
C6—C7—C2	121.5 (2)	C18—C17—C16	121.0 (2)
C6—C7—H7	119.3	C18—C17—H17	119.5
C2—C7—H7	119.3	C16—C17—H17	119.5
O1—C8—C9	108.69 (15)	C19—C18—C17	120.4 (2)
O1—C8—H8A	110.0	C19—C18—H18	119.8
C9—C8—H8A	110.0	C17—C18—H18	119.8
O1—C8—H8B	110.0	C20—C19—C18	119.1 (2)
C9—C8—H8B	110.0	C20—C19—H19	120.4
H8A—C8—H8B	108.3	C18—C19—H19	120.4
C10—C9—C14	118.49 (17)	C19—C20—C21	120.8 (2)
C10—C9—C8	123.42 (17)	C19—C20—H20	119.6
C14—C9—C8	118.09 (17)	C21—C20—H20	119.6
C11—C10—C9	120.55 (19)	C20—C21—C16	120.4 (2)
C11—C10—H10	119.7	C20—C21—H21	119.8
C9—C10—H10	119.7	C16—C21—H21	119.8
C12—C11—C10	120.6 (2)		

*Hydrogen-bond geometry (Å, °)*

Cg1, Cg2 and Cg3 are the centroids of the C2—C7, C9—C14 and C16—C21 rings, respectively.

<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>
C14—H14...O2 <sup>i</sup>	0.93	2.63	3.408 (3)	142
C4—H4...Cg3 <sup>ii</sup>	0.93	3.11	3.846 (3)	137
C13—H13...Cg3 <sup>i</sup>	0.93	2.88	3.653 (3)	141
C18—H18...Cg1 <sup>iii</sup>	0.93	3.20	3.820 (3)	126
C20—H20...Cg2 <sup>iv</sup>	0.93	2.96	3.651 (3)	132

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