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## Structure Reports

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## 2-Chloro-*N*-(3-chlorobenzoyl)benzene-sulfonamide

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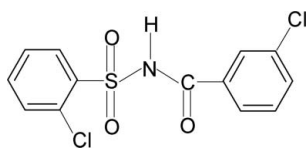
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Key indicators: single-crystal X-ray study;  $T = 299$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.054;  $wR$  factor = 0.154; data-to-parameter ratio = 15.5.

The asymmetric unit of the title compound,  $\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}_3\text{S}$ , contains two independent molecules. The conformation of the  $\text{C}=\text{O}$  bond is *anti* to the *meta*-Cl group in the chlorobenzoyl group of one of the molecules and *syn* in the other. The dihedral angles between the sulfonyl and benzoyl benzene rings are  $77.8$  (1) and  $83.5$  (1)°. In the crystal structure, two pairs of independent molecules are linked into a tetramer by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds.

### Related literature

For background literature and related structures, see: Gowda *et al.* (2009, 2010); Suchetan *et al.* (2010*a,b*).



### Experimental

#### Crystal data

 $\text{C}_{13}\text{H}_9\text{Cl}_2\text{NO}_3\text{S}$ 
 $M_r = 330.17$ 

 Triclinic,  $P\bar{1}$ 
 $a = 7.4399$  (6) Å

 $b = 11.679$  (1) Å

 $c = 17.138$  (2) Å

 $\alpha = 75.346$  (7)°

 $\beta = 83.188$  (8)°

 $\gamma = 77.732$  (7)°

 $V = 1404.5$  (2) Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.62$  mm<sup>-1</sup>  
 $T = 299$  K

 $0.20 \times 0.14 \times 0.08$  mm

#### Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2009)  
 $T_{\min} = 0.887$ ,  $T_{\max} = 0.952$   
 9768 measured reflections  
 5694 independent reflections  
 4267 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.054$ 
 $wR(F^2) = 0.154$ 
 $S = 1.04$ 

5694 reflections

367 parameters

2 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 1.10$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.50$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O6}$	0.84 (2)	2.02 (2)	2.836 (4)	162 (4)
$\text{N2}-\text{H2N}\cdots\text{O5}^i$	0.85 (2)	2.10 (2)	2.937 (4)	173 (4)

 Symmetry code: (i)  $-x + 2, -y + 1, -z + 1$ .

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5091).

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## supporting information

*Acta Cryst.* (2010). E66, o1343 [https://doi.org/10.1107/S1600536810016909]

**2-Chloro-*N*-(3-chlorobenzoyl)benzenesulfonamide****B. Thimme Gowda, Sabine Foro, P. A. Suchetan and Hartmut Fues****S1. Comment**

As a part of studying the effect of ring and the side chain substitutions on the crystal structures of *N*-aryl sulfonamides (Gowda *et al.*, 2009, 2010; Suchetan *et al.*, 2010*a,b*), the structure of 2-chloro-*N*-(3-chlorobenzoyl)-benzenesulfonamide (I) has been determined. The asymmetric unit of (I) contains two independent molecules. In the C—SO<sub>2</sub>—NH—C(O) segments, the N—H bonds are *anti* to the C=O bonds (Fig. 1), similar to those observed in 2-chloro-*N*-(3-methylbenzoyl)-benzenesulfonamide (II) (Suchetan *et al.*, 2010*b*), 2-methyl-*N*-(3-methylbenzoyl)-benzenesulfonamide (III) (Gowda *et al.*, 2010), 2-chloro-*N*-(2-chlorobenzoyl)-benzenesulfonamide (IV) (Suchetan *et al.*, 2010*a*), *N*-(benzoyl)-benzenesulfonamide (V) (Gowda *et al.*, 2009).

The conformation of the C=O bond is *anti* to the *meta*-Cl group in the benzoyl ring of one of the molecules and *syn* in the other, compared to the *anti* conformation observed between C=O bond and *meta*-methyl group in the benzoyl ring of (II).

The chlorobenzoyl and sulfonyl-bound chlorophenyl units in the two molecules of (I) are twisted with respect to the S—N bond, with torsional angles of -62.6 (3)° [C7—N1—S1—C1] and -62.6 (3)° [C20—N2—S2—C14], compared to those of -66.5 (2)° in (II), -66.2 (3)° in (III), -66.5 (2)° in (IV) and -66.9 (3)° in (V). The dihedral angles between the sulfonyl and the benzoyl-bound benzene rings are 77.8 (1)° (molecule 1) and 83.5 (1)° (molecule 2), compared to the values of 74.7 (1)° in (II), 74.8 (1)° in (III), 76.9 (1)° in (IV) and 80.3 (1)° in (V).

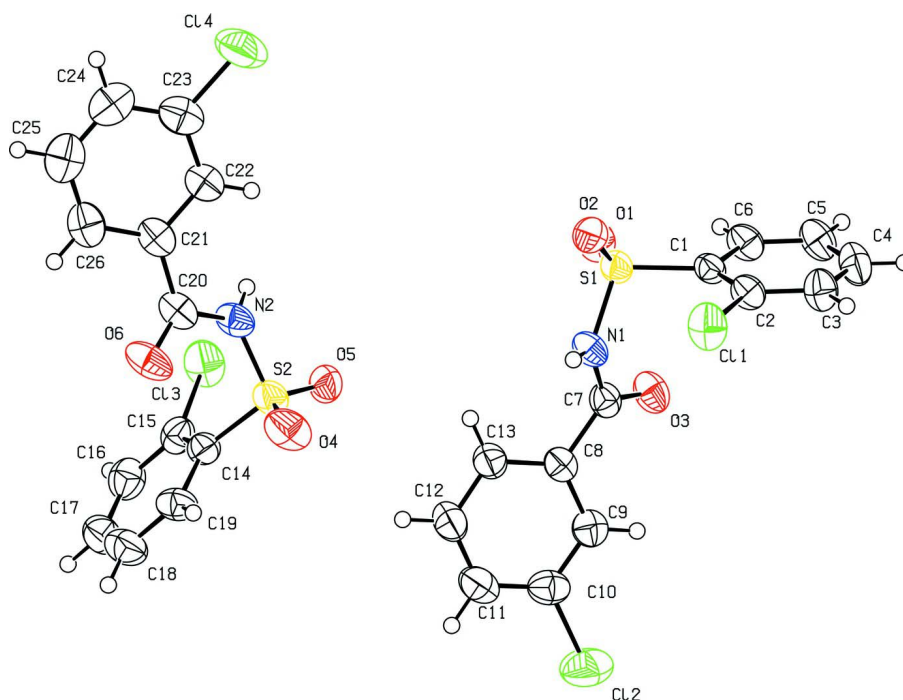
**S2. Experimental**

The title compound was prepared by refluxing a mixture of 3-chlorobenzoic acid, 2-chlorobenzenesulfonamide and phosphorous oxy chloride for 3 h on a water bath. The resultant mixture was cooled and poured into ice cold water. The solid obtained was filtered, washed thoroughly with water and then dissolved in sodium bicarbonate solution. The compound was later reprecipitated by acidifying the filtered solution with dilute HCl. It was filtered, dried and recrystallized. Rod like colourless single crystals of the title compound used in X-ray diffraction studies were obtained by a slow evaporation of its toluene solution at room temperature.

**S3. Refinement**

The H atoms of the NH groups were located in a difference map and refined with the a N—H distance restraint of 0.86 (2) %A. The other H atoms were positioned with idealized geometry using a riding model with C—H = 0.93 Å.

All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the  $U_{eq}$  of the parent atom). The residual electron-density features are located in the region of H25 and Cl4. The highest peak is 0.98 Å from H25 and the deepest hole is 0.68 Å from Cl4.



**Figure 1**

The two independent molecules of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

## 2-Chloro-*N*-(3-chlorobenzoyl)benzenesulfonamide

### Crystal data

$C_{13}H_9Cl_2NO_3S$

$M_r = 330.17$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.4399$  (6) Å

$b = 11.679$  (1) Å

$c = 17.138$  (2) Å

$\alpha = 75.346$  (7)°

$\beta = 83.188$  (8)°

$\gamma = 77.732$  (7)°

$V = 1404.5$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 672$

$D_x = 1.561$  Mg m<sup>-3</sup>

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

Cell parameters from 3572 reflections

$\theta = 2.5$ – $27.8$ °

$\mu = 0.62$  mm<sup>-1</sup>

$T = 299$  K

Rod, colourless

$0.20 \times 0.14 \times 0.08$  mm

### Data collection

Oxford Diffraction Xcalibur

diffractometer with a Sapphire CCD detector

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using  $\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.887$ ,  $T_{\max} = 0.952$

9768 measured reflections

5694 independent reflections

4267 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 26.4$ °,  $\theta_{\min} = 2.5$ °

$h = -9 \rightarrow 5$

$k = -14 \rightarrow 14$

$l = -19 \rightarrow 21$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.154$   
 $S = 1.04$   
 5694 reflections  
 367 parameters  
 2 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 1.64P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.014$   
 $\Delta\rho_{\max} = 1.10 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.50 \text{ e } \text{\AA}^{-3}$

*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.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2455 (4)	1.0034 (3)	0.13610 (19)	0.0380 (7)
C2	0.4149 (4)	1.0391 (3)	0.1159 (2)	0.0432 (8)
C3	0.4422 (5)	1.1225 (3)	0.0442 (2)	0.0543 (9)
H3	0.5556	1.1464	0.0304	0.065*
C4	0.3009 (6)	1.1700 (4)	-0.0067 (2)	0.0594 (10)
H4	0.3199	1.2258	-0.0548	0.071*
C5	0.1320 (5)	1.1358 (3)	0.0128 (2)	0.0564 (10)
H5	0.0372	1.1690	-0.0217	0.068*
C6	0.1041 (5)	1.0522 (3)	0.0839 (2)	0.0473 (8)
H6	-0.0095	1.0283	0.0970	0.057*
C7	0.3347 (4)	0.7053 (3)	0.1700 (2)	0.0421 (7)
C8	0.4322 (4)	0.5771 (3)	0.1922 (2)	0.0403 (7)
C9	0.5166 (5)	0.5225 (3)	0.1304 (2)	0.0488 (8)
H9	0.5157	0.5659	0.0768	0.059*
C10	0.6012 (5)	0.4034 (4)	0.1500 (3)	0.0539 (9)
C11	0.5995 (5)	0.3361 (4)	0.2282 (3)	0.0596 (10)
H11	0.6549	0.2550	0.2399	0.072*
C12	0.5148 (6)	0.3901 (4)	0.2892 (3)	0.0614 (10)
H12	0.5135	0.3450	0.3424	0.074*
C13	0.4315 (5)	0.5106 (3)	0.2723 (2)	0.0487 (8)
H13	0.3757	0.5468	0.3138	0.058*
N1	0.3355 (4)	0.7713 (2)	0.22646 (18)	0.0434 (7)
H1N	0.423 (4)	0.755 (3)	0.2573 (19)	0.052*
O1	0.0127 (3)	0.8835 (2)	0.22699 (17)	0.0600 (7)

O2	0.2495 (4)	0.9355 (2)	0.29433 (14)	0.0529 (6)
O3	0.2575 (4)	0.7488 (2)	0.10731 (15)	0.0548 (6)
S1	0.19546 (11)	0.90062 (8)	0.22791 (5)	0.0418 (2)
Cl1	0.59757 (13)	0.98058 (10)	0.17710 (6)	0.0621 (3)
Cl2	0.71150 (19)	0.33696 (12)	0.07272 (9)	0.0864 (4)
C14	0.7395 (4)	0.7963 (3)	0.4444 (2)	0.0418 (7)
C15	0.9034 (5)	0.8353 (3)	0.4444 (2)	0.0469 (8)
C16	0.9072 (6)	0.9573 (4)	0.4233 (2)	0.0573 (10)
H16	1.0162	0.9838	0.4240	0.069*
C17	0.7485 (7)	1.0391 (4)	0.4014 (3)	0.0648 (11)
H17	0.7510	1.1211	0.3875	0.078*
C18	0.5875 (6)	1.0018 (4)	0.3996 (3)	0.0633 (11)
H18	0.4816	1.0582	0.3841	0.076*
C19	0.5817 (5)	0.8804 (3)	0.4208 (2)	0.0506 (9)
H19	0.4722	0.8550	0.4193	0.061*
C20	0.7982 (5)	0.6143 (3)	0.3232 (2)	0.0473 (8)
C21	0.9079 (5)	0.5420 (3)	0.2688 (2)	0.0470 (8)
C22	0.9803 (5)	0.4209 (3)	0.2962 (2)	0.0511 (9)
H22	0.9681	0.3831	0.3507	0.061*
C23	1.0719 (5)	0.3567 (4)	0.2401 (3)	0.0597 (10)
C24	1.0906 (6)	0.4131 (5)	0.1593 (3)	0.0659 (11)
H24	1.1511	0.3691	0.1225	0.079*
C25	1.0212 (6)	0.5326 (5)	0.1332 (3)	0.0721 (12)
H25	1.0363	0.5703	0.0788	0.087*
C26	0.9289 (5)	0.5978 (4)	0.1869 (2)	0.0587 (10)
H26	0.8803	0.6793	0.1687	0.070*
N2	0.8416 (4)	0.5803 (3)	0.40323 (18)	0.0477 (7)
H2N	0.946 (3)	0.537 (3)	0.415 (2)	0.057*
O4	0.5315 (3)	0.6379 (3)	0.4726 (2)	0.0700 (8)
O5	0.8139 (3)	0.5845 (2)	0.54567 (15)	0.0547 (6)
O6	0.6750 (4)	0.6993 (2)	0.30102 (18)	0.0620 (8)
S2	0.71956 (11)	0.64315 (8)	0.47362 (6)	0.0466 (2)
Cl3	1.10996 (13)	0.73583 (10)	0.46678 (7)	0.0686 (3)
Cl4	1.1539 (2)	0.20474 (11)	0.27335 (10)	0.0915 (4)

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0388 (16)	0.0328 (16)	0.0392 (17)	-0.0003 (13)	-0.0070 (13)	-0.0059 (13)
C2	0.0401 (18)	0.0421 (18)	0.0462 (19)	-0.0046 (14)	-0.0122 (14)	-0.0067 (15)
C3	0.054 (2)	0.054 (2)	0.053 (2)	-0.0187 (18)	-0.0060 (17)	-0.0012 (17)
C4	0.075 (3)	0.048 (2)	0.049 (2)	-0.0125 (19)	-0.0116 (19)	0.0042 (17)
C5	0.058 (2)	0.050 (2)	0.053 (2)	-0.0010 (18)	-0.0241 (18)	0.0023 (17)
C6	0.0389 (18)	0.0459 (19)	0.055 (2)	-0.0031 (15)	-0.0151 (15)	-0.0060 (16)
C7	0.0380 (17)	0.0400 (18)	0.0467 (19)	-0.0116 (14)	-0.0031 (14)	-0.0040 (14)
C8	0.0340 (16)	0.0381 (17)	0.0496 (19)	-0.0107 (13)	-0.0064 (14)	-0.0067 (14)
C9	0.050 (2)	0.048 (2)	0.051 (2)	-0.0133 (16)	-0.0048 (16)	-0.0118 (16)
C10	0.047 (2)	0.051 (2)	0.069 (3)	-0.0105 (17)	-0.0015 (18)	-0.0247 (19)

C11	0.054 (2)	0.042 (2)	0.078 (3)	-0.0032 (17)	-0.006 (2)	-0.0086 (19)
C12	0.063 (2)	0.047 (2)	0.062 (3)	-0.0045 (19)	-0.003 (2)	0.0032 (19)
C13	0.0467 (19)	0.0434 (19)	0.052 (2)	-0.0079 (15)	-0.0009 (16)	-0.0050 (16)
N1	0.0409 (15)	0.0375 (15)	0.0500 (17)	-0.0019 (12)	-0.0174 (12)	-0.0052 (13)
O1	0.0351 (13)	0.0638 (17)	0.0706 (18)	-0.0073 (12)	-0.0041 (12)	0.0016 (13)
O2	0.0630 (16)	0.0529 (15)	0.0388 (13)	-0.0027 (12)	-0.0037 (11)	-0.0104 (11)
O3	0.0632 (16)	0.0486 (14)	0.0504 (15)	-0.0082 (12)	-0.0212 (12)	-0.0019 (11)
S1	0.0359 (4)	0.0405 (4)	0.0432 (5)	-0.0018 (3)	-0.0037 (3)	-0.0033 (3)
Cl1	0.0421 (5)	0.0781 (7)	0.0618 (6)	-0.0153 (4)	-0.0194 (4)	0.0017 (5)
Cl2	0.0947 (9)	0.0792 (8)	0.0946 (9)	-0.0088 (7)	0.0062 (7)	-0.0494 (7)
C14	0.0397 (17)	0.0442 (18)	0.0381 (17)	-0.0008 (14)	-0.0055 (13)	-0.0082 (14)
C15	0.0420 (18)	0.058 (2)	0.0384 (18)	-0.0080 (16)	-0.0051 (14)	-0.0075 (16)
C16	0.063 (2)	0.062 (2)	0.051 (2)	-0.022 (2)	-0.0014 (18)	-0.0133 (18)
C17	0.087 (3)	0.046 (2)	0.059 (2)	-0.008 (2)	-0.006 (2)	-0.0116 (18)
C18	0.066 (3)	0.052 (2)	0.067 (3)	0.008 (2)	-0.017 (2)	-0.014 (2)
C19	0.0440 (19)	0.052 (2)	0.056 (2)	0.0047 (16)	-0.0138 (16)	-0.0199 (17)
C20	0.0471 (19)	0.0395 (18)	0.059 (2)	-0.0079 (15)	-0.0202 (16)	-0.0107 (16)
C21	0.0423 (18)	0.0457 (19)	0.056 (2)	-0.0091 (15)	-0.0205 (16)	-0.0082 (16)
C22	0.052 (2)	0.046 (2)	0.058 (2)	-0.0081 (16)	-0.0127 (17)	-0.0133 (17)
C23	0.051 (2)	0.051 (2)	0.083 (3)	-0.0113 (18)	-0.012 (2)	-0.022 (2)
C24	0.057 (2)	0.086 (3)	0.066 (3)	-0.024 (2)	0.001 (2)	-0.032 (2)
C25	0.072 (3)	0.086 (3)	0.060 (3)	-0.027 (3)	-0.006 (2)	-0.010 (2)
C26	0.056 (2)	0.060 (2)	0.060 (2)	-0.0166 (19)	-0.0180 (19)	-0.0027 (19)
N2	0.0421 (16)	0.0456 (17)	0.0520 (18)	0.0066 (13)	-0.0206 (13)	-0.0100 (13)
O4	0.0343 (13)	0.0585 (17)	0.112 (2)	-0.0072 (12)	-0.0075 (14)	-0.0100 (16)
O5	0.0500 (14)	0.0572 (15)	0.0441 (14)	0.0009 (12)	-0.0030 (11)	0.0020 (11)
O6	0.0612 (16)	0.0461 (15)	0.0787 (19)	0.0104 (12)	-0.0416 (14)	-0.0149 (13)
S2	0.0334 (4)	0.0445 (5)	0.0555 (5)	-0.0009 (3)	-0.0062 (4)	-0.0041 (4)
Cl3	0.0357 (5)	0.0757 (7)	0.0822 (7)	-0.0091 (4)	-0.0112 (4)	0.0057 (5)
Cl4	0.1048 (10)	0.0482 (6)	0.1177 (11)	0.0030 (6)	-0.0070 (8)	-0.0277 (7)

*Geometric parameters (Å, °)*

C1—C2	1.389 (5)	C14—C19	1.388 (5)
C1—C6	1.394 (4)	C14—C15	1.390 (5)
C1—S1	1.775 (3)	C14—S2	1.765 (4)
C2—C3	1.386 (5)	C15—C16	1.384 (5)
C2—Cl1	1.730 (3)	C15—Cl3	1.736 (4)
C3—C4	1.377 (5)	C16—C17	1.375 (6)
C3—H3	0.93	C16—H16	0.93
C4—C5	1.377 (6)	C17—C18	1.365 (6)
C4—H4	0.93	C17—H17	0.93
C5—C6	1.381 (5)	C18—C19	1.380 (6)
C5—H5	0.93	C18—H18	0.93
C6—H6	0.93	C19—H19	0.93
C7—O3	1.220 (4)	C20—O6	1.214 (4)
C7—N1	1.382 (4)	C20—N2	1.384 (5)
C7—C8	1.493 (5)	C20—C21	1.475 (5)

C8—C9	1.391 (5)	C21—C22	1.382 (5)
C8—C13	1.396 (5)	C21—C26	1.396 (5)
C9—C10	1.374 (5)	C22—C23	1.393 (6)
C9—H9	0.93	C22—H22	0.93
C10—C11	1.372 (6)	C23—C24	1.379 (6)
C10—C12	1.738 (4)	C23—C14	1.719 (4)
C11—C12	1.377 (6)	C24—C25	1.359 (7)
C11—H11	0.93	C24—H24	0.93
C12—C13	1.383 (5)	C25—C26	1.371 (6)
C12—H12	0.93	C25—H25	0.93
C13—H13	0.93	C26—H26	0.93
N1—S1	1.647 (3)	N2—S2	1.650 (3)
N1—H1N	0.845 (18)	N2—H2N	0.846 (19)
O1—S1	1.418 (3)	O4—S2	1.416 (3)
O2—S1	1.427 (3)	O5—S2	1.435 (3)
C2—C1—C6	119.5 (3)	C19—C14—C15	119.4 (3)
C2—C1—S1	123.1 (2)	C19—C14—S2	117.3 (3)
C6—C1—S1	117.3 (3)	C15—C14—S2	123.2 (3)
C3—C2—C1	119.9 (3)	C16—C15—C14	120.0 (3)
C3—C2—C11	118.1 (3)	C16—C15—C13	117.6 (3)
C1—C2—C11	122.0 (3)	C14—C15—C13	122.4 (3)
C4—C3—C2	119.9 (4)	C17—C16—C15	119.5 (4)
C4—C3—H3	120.1	C17—C16—H16	120.2
C2—C3—H3	120.1	C15—C16—H16	120.2
C5—C4—C3	120.8 (4)	C18—C17—C16	121.0 (4)
C5—C4—H4	119.6	C18—C17—H17	119.5
C3—C4—H4	119.6	C16—C17—H17	119.5
C4—C5—C6	119.7 (3)	C17—C18—C19	120.0 (4)
C4—C5—H5	120.1	C17—C18—H18	120.0
C6—C5—H5	120.1	C19—C18—H18	120.0
C5—C6—C1	120.2 (3)	C18—C19—C14	120.0 (4)
C5—C6—H6	119.9	C18—C19—H19	120.0
C1—C6—H6	119.9	C14—C19—H19	120.0
O3—C7—N1	122.1 (3)	O6—C20—N2	120.3 (3)
O3—C7—C8	122.8 (3)	O6—C20—C21	123.3 (3)
N1—C7—C8	115.0 (3)	N2—C20—C21	116.4 (3)
C9—C8—C13	120.1 (3)	C22—C21—C26	120.2 (4)
C9—C8—C7	118.4 (3)	C22—C21—C20	121.8 (3)
C13—C8—C7	121.4 (3)	C26—C21—C20	117.9 (3)
C10—C9—C8	118.8 (4)	C21—C22—C23	118.5 (4)
C10—C9—H9	120.6	C21—C22—H22	120.8
C8—C9—H9	120.6	C23—C22—H22	120.8
C9—C10—C11	121.9 (4)	C24—C23—C22	120.6 (4)
C9—C10—C12	118.5 (3)	C24—C23—C14	120.8 (4)
C11—C10—C12	119.6 (3)	C22—C23—C14	118.6 (3)
C12—C11—C10	119.2 (4)	C25—C24—C23	120.5 (4)
C12—C11—H11	120.4	C25—C24—H24	119.7

C10—C11—H11	120.4	C23—C24—H24	119.7
C11—C12—C13	120.8 (4)	C24—C25—C26	120.2 (4)
C11—C12—H12	119.6	C24—C25—H25	119.9
C13—C12—H12	119.6	C26—C25—H25	119.9
C12—C13—C8	119.2 (4)	C25—C26—C21	120.1 (4)
C12—C13—H13	120.4	C25—C26—H26	119.9
C8—C13—H13	120.4	C21—C26—H26	119.9
C7—N1—S1	123.8 (2)	C20—N2—S2	122.5 (2)
C7—N1—H1N	121 (3)	C20—N2—H2N	119 (3)
S1—N1—H1N	114 (3)	S2—N2—H2N	117 (3)
O1—S1—O2	120.43 (17)	O4—S2—O5	119.14 (18)
O1—S1—N1	107.77 (16)	O4—S2—N2	109.45 (18)
O2—S1—N1	103.83 (15)	O5—S2—N2	104.14 (15)
O1—S1—C1	107.48 (16)	O4—S2—C14	107.70 (16)
O2—S1—C1	109.82 (15)	O5—S2—C14	110.08 (16)
N1—S1—C1	106.73 (15)	N2—S2—C14	105.52 (16)
C6—C1—C2—C3	-0.2 (5)	C19—C14—C15—C16	2.0 (5)
S1—C1—C2—C3	-178.1 (3)	S2—C14—C15—C16	-177.8 (3)
C6—C1—C2—C11	-179.0 (3)	C19—C14—C15—C13	-175.8 (3)
S1—C1—C2—C11	3.1 (4)	S2—C14—C15—C13	4.5 (4)
C1—C2—C3—C4	0.2 (6)	C14—C15—C16—C17	-1.0 (6)
C11—C2—C3—C4	179.1 (3)	C13—C15—C16—C17	176.9 (3)
C2—C3—C4—C5	0.2 (6)	C15—C16—C17—C18	-0.4 (6)
C3—C4—C5—C6	-0.6 (6)	C16—C17—C18—C19	0.6 (7)
C4—C5—C6—C1	0.7 (6)	C17—C18—C19—C14	0.4 (6)
C2—C1—C6—C5	-0.3 (5)	C15—C14—C19—C18	-1.7 (5)
S1—C1—C6—C5	177.7 (3)	S2—C14—C19—C18	178.1 (3)
O3—C7—C8—C9	31.9 (5)	O6—C20—C21—C22	-149.0 (4)
N1—C7—C8—C9	-149.0 (3)	N2—C20—C21—C22	30.7 (5)
O3—C7—C8—C13	-144.7 (4)	O6—C20—C21—C26	27.5 (5)
N1—C7—C8—C13	34.4 (4)	N2—C20—C21—C26	-152.8 (3)
C13—C8—C9—C10	-1.1 (5)	C26—C21—C22—C23	-0.7 (5)
C7—C8—C9—C10	-177.8 (3)	C20—C21—C22—C23	175.8 (3)
C8—C9—C10—C11	2.2 (6)	C21—C22—C23—C24	0.4 (6)
C8—C9—C10—C12	-178.3 (3)	C21—C22—C23—C14	-177.4 (3)
C9—C10—C11—C12	-1.7 (6)	C22—C23—C24—C25	0.5 (6)
C12—C10—C11—C12	178.8 (3)	C14—C23—C24—C25	178.3 (3)
C10—C11—C12—C13	0.2 (6)	C23—C24—C25—C26	-1.1 (7)
C11—C12—C13—C8	0.8 (6)	C24—C25—C26—C21	0.8 (6)
C9—C8—C13—C12	-0.3 (5)	C22—C21—C26—C25	0.1 (5)
C7—C8—C13—C12	176.3 (3)	C20—C21—C26—C25	-176.5 (3)
O3—C7—N1—S1	15.6 (5)	O6—C20—N2—S2	5.7 (5)
C8—C7—N1—S1	-163.5 (2)	C21—C20—N2—S2	-173.9 (2)
C7—N1—S1—O1	52.6 (3)	C20—N2—S2—O4	53.1 (3)
C7—N1—S1—O2	-178.6 (3)	C20—N2—S2—O5	-178.5 (3)
C7—N1—S1—C1	-62.6 (3)	C20—N2—S2—C14	-62.6 (3)
C2—C1—S1—O1	-178.8 (3)	C19—C14—S2—O4	-4.5 (3)



C6—C1—S1—O1	3.3 (3)	C15—C14—S2—O4	175.2 (3)
C2—C1—S1—O2	48.6 (3)	C19—C14—S2—O5	-135.9 (3)
C6—C1—S1—O2	-129.4 (3)	C15—C14—S2—O5	43.9 (3)
C2—C1—S1—N1	-63.4 (3)	C19—C14—S2—N2	112.3 (3)
C6—C1—S1—N1	118.7 (3)	C15—C14—S2—N2	-67.9 (3)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1N $\cdots$ O6	0.84 (2)	2.02 (2)	2.836 (4)	162 (4)
N2—H2N $\cdots$ O5 <sup>i</sup>	0.85 (2)	2.10 (2)	2.937 (4)	173 (4)

Symmetry code: (i)  $-x+2, -y+1, -z+1$ .