

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-Chloro-6-(2,3-dichlorobenzene-sulfonamido)benzoic acid

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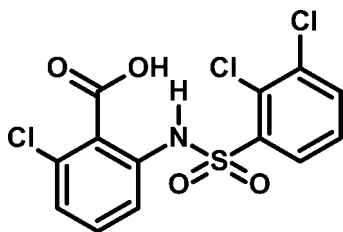
Received 24 April 2013; accepted 27 April 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.038; wR factor = 0.104; data-to-parameter ratio = 15.0.

In the title compound, $\text{C}_{13}\text{H}_8\text{Cl}_3\text{NO}_4\text{S}$, the aromatic rings are oriented at a dihedral angle of $68.94(1)^\circ$ and the molecule adopts a V-shape. An intramolecular $\text{N}-\text{H}\cdots\text{O}$ interaction generates a six-membered $S(6)$ ring motif. In the crystal, pairs of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds involving the carboxy group link the molecules into inversion dimers with an $R_2^2(8)$ motif. $\text{N}-\text{H}\cdots\text{O}$ and non-classical $\text{C}-\text{H}\cdots\text{O}$ interactions connect the molecules, forming sheets propagating in (100).

Related literature

For the synthesis, see: Arshad *et al.* (2012) For related structures, see: Arshad *et al.* (2009, 2011). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{13}\text{H}_8\text{Cl}_3\text{NO}_4\text{S}$
 $M_r = 380.61$
Monoclinic, $P2_1/c$

$a = 9.0164(3)$ Å
 $b = 18.6017(5)$ Å
 $c = 9.8574(3)$ Å

$\beta = 111.653(3)^\circ$
 $V = 1536.62(8)$ Å³
 $Z = 4$
Cu $K\alpha$ radiation

$\mu = 6.83$ mm⁻¹
 $T = 296$ K
 $0.38 \times 0.20 \times 0.18$ mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
 $T_{\min} = 0.467$, $T_{\max} = 1.000$

11742 measured reflections
3018 independent reflections
2597 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.104$
 $S = 1.04$
3018 reflections

201 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.55$ e Å⁻³
 $\Delta\rho_{\min} = -0.60$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{O3}$	0.86	2.55	2.940 (2)	108
$\text{C12}-\text{H12}\cdots\text{O3}^i$	0.93	2.59	3.425 (3)	150
$\text{O3}-\text{H3}\cdots\text{O4}^{ii}$	0.82	1.85	2.666 (2)	176
$\text{N1}-\text{H1}\cdots\text{O2}^{iii}$	0.86	2.30	3.128 (2)	162
$\text{C5}-\text{H5}\cdots\text{O4}^{iv}$	0.93	2.53	3.256 (4)	135
$\text{C10}-\text{H10}\cdots\text{O1}^v$	0.93	2.51	3.165 (3)	127

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

Data collection: *CrysAlis PRO* (Agilent, 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: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *X-SEED* (Barbour, 2001).

The authors would like to thank the Deanship of Scientific Research at King Abdulaziz University for the support of this research *via* the Research Group Track of Grant No. (3-102/428).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG5312).

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supporting information

Acta Cryst. (2013). E69, o832 [doi:10.1107/S1600536813011574]

2-Chloro-6-(2,3-dichlorobenzenesulfonamido)benzoic acid

Ayesha Munir, Hafiz Mubashar-ur-Rehman, Abdullah M. Asiri, Islam Ullah Khan and Muhammad Nadeem Arshad

S1. Comment

In connection to synthesis of halogenated sulfonamide derivatives 2-Chloro-4-(2-iodobenzenesulfonamido)benzoic acid (Arshad *et al.*, 2011) and 2-Chloro-5-(2-iodobenzenesulfonamido)benzoic acid (Arshad *et al.*, 2009), we are reporting the crystal structure of title compound.

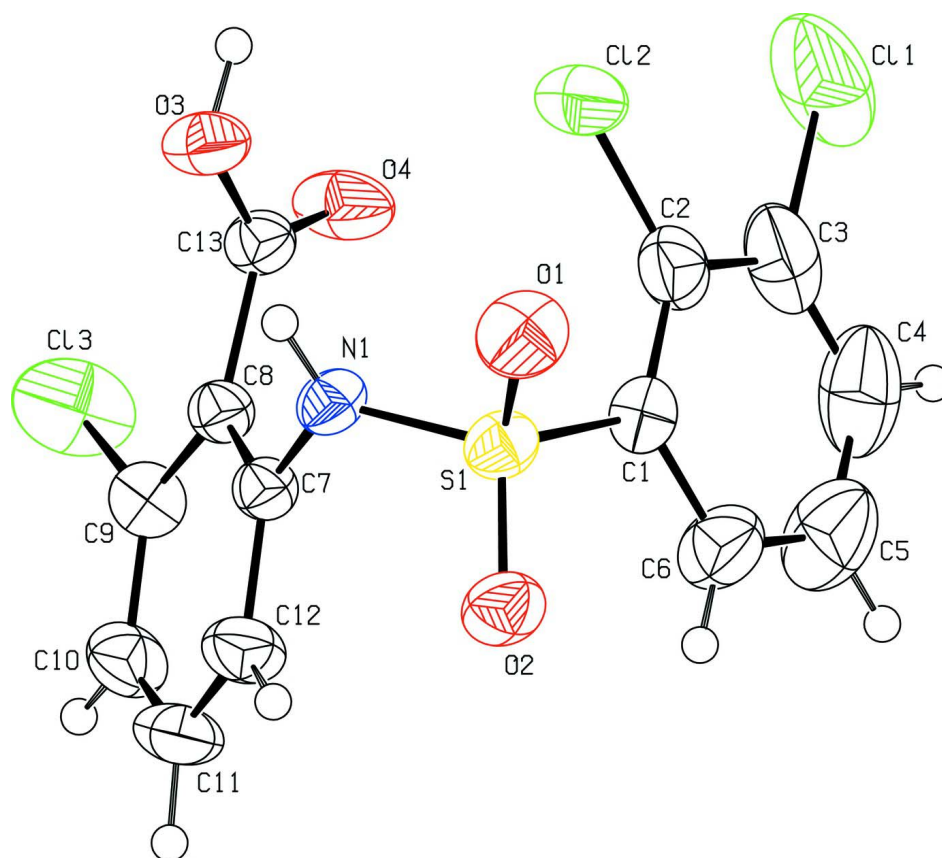
The two aromatic rings [(C1—C6) & (C7—C12)] in the structure of molecule are oriented at dihedral angle of 68.94 (1)°. The carboxylic group (C13/O3/O4) is twisted at 58.11 (1)° with respect to its mother aromatic ring (C7—C12) and its atoms C13, O3 & O4 are away by -0.1938 (35)Å, 0.6924 (39)Å, -1.1739 (39)Å respectively from the mean plane generating from atoms C7/C8/C9/C10/C11/C12 with the r.m.s deviation of 0.0183 (15) Å. The amino and carboxylic groups are involved in classical N1—H1···O3 intramolecular hydrogen bonding interaction and produce six membered ring motif S^1_1 (6) (Bernstein *et al.* 1995) which is oriented at dihedral angles of 54.30 (11)° & 18.98 (12)° with respect to two aromatic rings [(C1—C6) & (C7—C12)], respectively. On the other hand the amino group get connected with oxygen of SO₂ to form intermolecular N1—H1···O2 hydrogen bond. The carboxylic group gives typical inversion dimerization by generating eight membered ring motif R^2_2 (8) (Bernstein *et al.* 1995) through O3—H3···O4 interaction. The non-classical C—H···O type interaction have also been observed in the molecule (Fig. 2) for which symmetry detail are available in Table 1.

S2. Experimental

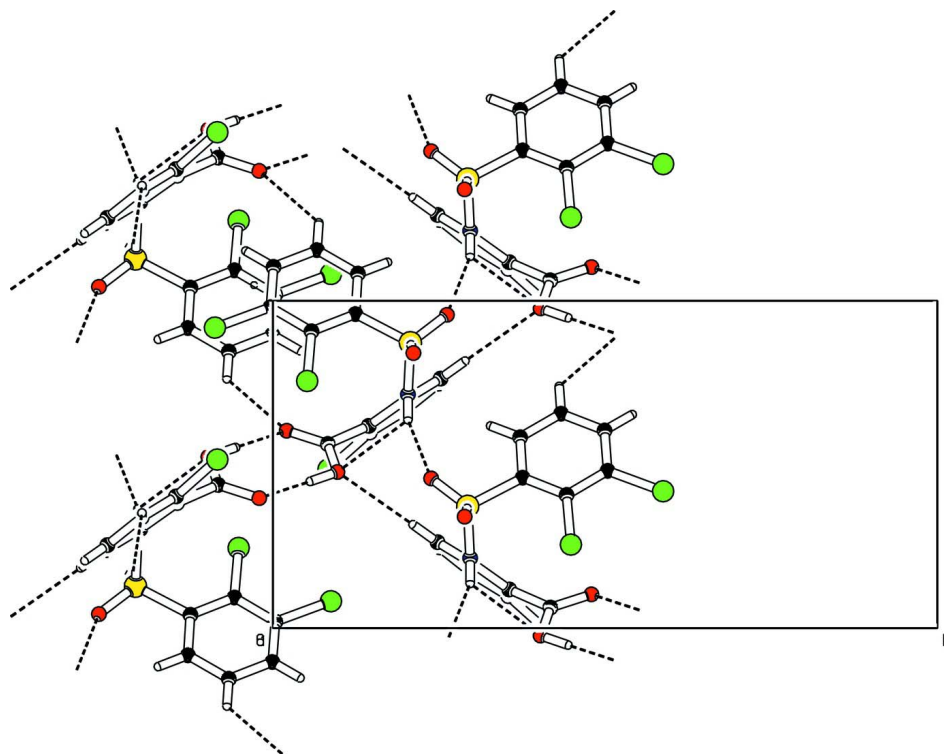
The title compound was synthesised following the literature method (Arshad *et al.*, 2012) and recrystallized from ethyl-acetate under slow evaporation at room temperature.

S3. Refinement

All the H-atoms were positioned with idealized geometry with C—H = 0.93 Å, N—H = 0.86 Å, O—H = 0.82 Å and were refined as riding with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{K})$, where K = C, N & O for all H-atoms. The reflections (0 1 2), (1 3 1), (1 0 0), (2 1 0) & (0 2 0) are omitted in final refinement.

**Figure 1**

The labelled structure of (C₁₃ H₈ Cl₃ N O₄ S) with 50% probability of thermal ellipsoids.

**Figure 2**

A perspective view showing two dimensional network generating through O—H···O, N—H···O and C—H···O hydrogen bonds, drawn using dashed lines.

2-Chloro-6-(2,3-dichlorobenzenesulfonamido)benzoic acid

Crystal data

$C_{13}H_8Cl_3NO_4S$

$M_r = 380.61$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 9.0164\ (3)\ \text{\AA}$

$b = 18.6017\ (5)\ \text{\AA}$

$c = 9.8574\ (3)\ \text{\AA}$

$\beta = 111.653\ (3)^\circ$

$V = 1536.62\ (8)\ \text{\AA}^3$

$Z = 4$

$F(000) = 768$

$D_x = 1.645\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54184\ \text{\AA}$

Cell parameters from 5339 reflections

$\theta = 4.8\text{--}73.0^\circ$

$\mu = 6.83\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Prismatic, colorless

$0.38 \times 0.20 \times 0.18\ \text{mm}$

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas, CCD)

diffractometer

Radiation source: SuperNova (Cu) X-ray

Source

Mirror monochromator

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Agilent, 2012)

$T_{\min} = 0.467$, $T_{\max} = 1.000$

11742 measured reflections

3018 independent reflections

2597 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 73.1^\circ$, $\theta_{\min} = 5.4^\circ$

$h = -10 \rightarrow 11$

$k = -22 \rightarrow 22$

$l = -12 \rightarrow 11$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.104$
 $S = 1.04$
 3018 reflections
 201 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
 $w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 1.0131P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.55 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.60 \text{ e } \text{Å}^{-3}$
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.0022 (2)

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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.21203 (15)	0.41272 (5)	0.58195 (14)	0.1161 (5)
Cl2	0.17428 (9)	0.55156 (5)	0.74492 (8)	0.0718 (3)
Cl3	0.94473 (9)	0.58369 (5)	1.01517 (11)	0.0797 (3)
S1	0.24536 (6)	0.70690 (3)	0.62789 (6)	0.03763 (17)
O1	0.1045 (2)	0.71147 (11)	0.6596 (2)	0.0562 (5)
O2	0.2792 (2)	0.76184 (9)	0.54279 (18)	0.0482 (4)
O3	0.5137 (2)	0.59728 (8)	1.02304 (19)	0.0460 (4)
H3	0.4816	0.5600	1.0473	0.055*
O4	0.6012 (2)	0.52066 (9)	0.8971 (2)	0.0572 (5)
N1	0.3928 (2)	0.70318 (10)	0.78616 (19)	0.0357 (4)
H1	0.3706	0.7032	0.8638	0.043*
C1	0.2524 (3)	0.62421 (13)	0.5405 (2)	0.0417 (5)
C2	0.2255 (3)	0.55805 (14)	0.5932 (3)	0.0510 (6)
C3	0.2403 (4)	0.49629 (16)	0.5195 (4)	0.0693 (9)
C4	0.2779 (4)	0.5009 (2)	0.3962 (4)	0.0843 (11)
H4	0.2867	0.4592	0.3476	0.101*
C5	0.3022 (5)	0.5663 (2)	0.3450 (4)	0.0804 (10)
H5	0.3269	0.5691	0.2615	0.096*
C6	0.2903 (4)	0.62797 (17)	0.4168 (3)	0.0583 (7)
H6	0.3078	0.6724	0.3823	0.070*
C7	0.5563 (2)	0.69989 (11)	0.8019 (2)	0.0327 (4)
C8	0.6539 (2)	0.64427 (11)	0.8821 (2)	0.0329 (4)
C9	0.8156 (3)	0.64584 (13)	0.9024 (3)	0.0418 (5)

C10	0.8775 (3)	0.69735 (14)	0.8382 (3)	0.0485 (6)
H10	0.9852	0.6970	0.8518	0.058*
C11	0.7777 (3)	0.74919 (15)	0.7535 (3)	0.0536 (7)
H11	0.8175	0.7829	0.7061	0.064*
C12	0.6188 (3)	0.75223 (13)	0.7376 (3)	0.0467 (6)
H12	0.5540	0.7892	0.6840	0.056*
C13	0.5870 (3)	0.58240 (11)	0.9374 (2)	0.0348 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.1280 (9)	0.0446 (5)	0.1266 (9)	-0.0192 (5)	-0.0106 (7)	0.0082 (5)
C12	0.0734 (5)	0.0782 (5)	0.0597 (4)	-0.0271 (4)	0.0197 (3)	0.0177 (4)
C13	0.0502 (4)	0.0720 (5)	0.1115 (7)	0.0207 (3)	0.0236 (4)	0.0361 (5)
S1	0.0363 (3)	0.0420 (3)	0.0365 (3)	0.0046 (2)	0.0158 (2)	0.0039 (2)
O1	0.0388 (9)	0.0760 (13)	0.0587 (11)	0.0094 (8)	0.0238 (8)	0.0034 (9)
O2	0.0531 (9)	0.0456 (10)	0.0438 (9)	0.0048 (7)	0.0153 (7)	0.0123 (7)
O3	0.0692 (11)	0.0324 (8)	0.0514 (10)	-0.0026 (8)	0.0397 (9)	0.0004 (7)
O4	0.0914 (14)	0.0287 (8)	0.0748 (13)	-0.0047 (8)	0.0580 (11)	-0.0055 (8)
N1	0.0380 (9)	0.0422 (10)	0.0303 (9)	0.0018 (7)	0.0167 (7)	0.0005 (7)
C1	0.0419 (11)	0.0449 (13)	0.0356 (11)	-0.0006 (10)	0.0111 (9)	-0.0023 (9)
C2	0.0446 (13)	0.0496 (15)	0.0468 (14)	-0.0081 (11)	0.0027 (11)	0.0017 (11)
C3	0.0639 (17)	0.0444 (16)	0.072 (2)	-0.0044 (13)	-0.0075 (15)	-0.0037 (14)
C4	0.095 (2)	0.070 (2)	0.070 (2)	0.0129 (19)	0.0098 (19)	-0.0296 (18)
C5	0.108 (3)	0.078 (2)	0.0594 (19)	0.012 (2)	0.0362 (19)	-0.0156 (17)
C6	0.0753 (18)	0.0590 (17)	0.0460 (14)	0.0016 (14)	0.0285 (13)	-0.0020 (12)
C7	0.0369 (10)	0.0302 (10)	0.0325 (10)	-0.0020 (8)	0.0148 (8)	-0.0012 (8)
C8	0.0405 (10)	0.0270 (10)	0.0336 (10)	-0.0026 (8)	0.0166 (8)	-0.0021 (8)
C9	0.0396 (11)	0.0391 (12)	0.0474 (13)	0.0024 (9)	0.0168 (10)	0.0002 (10)
C10	0.0369 (11)	0.0556 (15)	0.0568 (15)	-0.0089 (10)	0.0218 (11)	-0.0030 (12)
C11	0.0518 (14)	0.0530 (16)	0.0602 (16)	-0.0145 (11)	0.0257 (12)	0.0121 (12)
C12	0.0468 (13)	0.0401 (13)	0.0515 (14)	-0.0042 (10)	0.0161 (11)	0.0126 (10)
C13	0.0418 (11)	0.0297 (10)	0.0357 (11)	0.0013 (8)	0.0174 (9)	0.0012 (8)

Geometric parameters (Å, °)

C11—C3	1.725 (3)	C4—C5	1.366 (5)
C12—C2	1.725 (3)	C4—H4	0.9300
C13—C9	1.724 (2)	C5—C6	1.373 (4)
S1—O1	1.4179 (17)	C5—H5	0.9300
S1—O2	1.4247 (17)	C6—H6	0.9300
S1—N1	1.6357 (18)	C7—C12	1.389 (3)
S1—C1	1.776 (2)	C7—C8	1.399 (3)
O3—C13	1.279 (3)	C8—C9	1.397 (3)
O3—H3	0.8200	C8—C13	1.493 (3)
O4—C13	1.238 (3)	C9—C10	1.375 (3)
N1—C7	1.426 (3)	C10—C11	1.372 (4)
N1—H1	0.8600	C10—H10	0.9300

C1—C6	1.384 (3)	C11—C12	1.383 (3)
C1—C2	1.391 (3)	C11—H11	0.9300
C2—C3	1.391 (4)	C12—H12	0.9300
C3—C4	1.380 (5)		
O1—S1—O2	119.37 (11)	C5—C6—C1	120.3 (3)
O1—S1—N1	105.73 (10)	C5—C6—H6	119.9
O2—S1—N1	108.47 (10)	C1—C6—H6	119.9
O1—S1—C1	110.74 (12)	C12—C7—C8	120.0 (2)
O2—S1—C1	106.38 (11)	C12—C7—N1	119.82 (19)
N1—S1—C1	105.32 (10)	C8—C7—N1	120.19 (18)
C13—O3—H3	109.5	C9—C8—C7	118.12 (19)
C7—N1—S1	123.33 (14)	C9—C8—C13	120.35 (19)
C7—N1—H1	118.3	C7—C8—C13	121.44 (18)
S1—N1—H1	118.3	C10—C9—C8	121.9 (2)
C6—C1—C2	120.5 (2)	C10—C9—C13	118.17 (18)
C6—C1—S1	116.6 (2)	C8—C9—C13	119.94 (18)
C2—C1—S1	122.88 (19)	C11—C10—C9	118.9 (2)
C1—C2—C3	118.2 (3)	C11—C10—H10	120.5
C1—C2—C12	121.7 (2)	C9—C10—H10	120.5
C3—C2—C12	120.2 (2)	C10—C11—C12	121.2 (2)
C4—C3—C2	120.7 (3)	C10—C11—H11	119.4
C4—C3—C11	119.1 (3)	C12—C11—H11	119.4
C2—C3—C11	120.2 (3)	C11—C12—C7	119.8 (2)
C5—C4—C3	120.4 (3)	C11—C12—H12	120.1
C5—C4—H4	119.8	C7—C12—H12	120.1
C3—C4—H4	119.8	O4—C13—O3	123.6 (2)
C4—C5—C6	120.0 (3)	O4—C13—C8	119.58 (19)
C4—C5—H5	120.0	O3—C13—C8	116.82 (18)
C6—C5—H5	120.0		
O1—S1—N1—C7	-178.47 (17)	S1—C1—C6—C5	178.3 (3)
O2—S1—N1—C7	-49.3 (2)	S1—N1—C7—C12	55.1 (3)
C1—S1—N1—C7	64.24 (19)	S1—N1—C7—C8	-125.01 (19)
O1—S1—C1—C6	132.5 (2)	C12—C7—C8—C9	3.9 (3)
O2—S1—C1—C6	1.4 (2)	N1—C7—C8—C9	-175.94 (19)
N1—S1—C1—C6	-113.6 (2)	C12—C7—C8—C13	-172.5 (2)
O1—S1—C1—C2	-49.0 (2)	N1—C7—C8—C13	7.6 (3)
O2—S1—C1—C2	179.83 (19)	C7—C8—C9—C10	-4.4 (3)
N1—S1—C1—C2	64.8 (2)	C13—C8—C9—C10	172.1 (2)
C6—C1—C2—C3	1.0 (4)	C7—C8—C9—C13	173.60 (17)
S1—C1—C2—C3	-177.45 (19)	C13—C8—C9—C13	-9.9 (3)
C6—C1—C2—C12	-178.7 (2)	C8—C9—C10—C11	1.0 (4)
S1—C1—C2—C12	2.9 (3)	C13—C9—C10—C11	-177.0 (2)
C1—C2—C3—C4	-1.1 (4)	C9—C10—C11—C12	3.0 (4)
C12—C2—C3—C4	178.6 (2)	C10—C11—C12—C7	-3.4 (4)
C1—C2—C3—C11	178.77 (19)	C8—C7—C12—C11	-0.2 (4)
C12—C2—C3—C11	-1.5 (3)	N1—C7—C12—C11	179.7 (2)

C2—C3—C4—C5	0.4 (5)	C9—C8—C13—O4	-56.9 (3)
C11—C3—C4—C5	-179.4 (3)	C7—C8—C13—O4	119.5 (2)
C3—C4—C5—C6	0.4 (6)	C9—C8—C13—O3	124.7 (2)
C4—C5—C6—C1	-0.5 (5)	C7—C8—C13—O3	-58.9 (3)
C2—C1—C6—C5	-0.2 (4)		

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>
N1—H1...O3	0.86	2.55	2.940 (2)	108
C12—H12...O3 ⁱ	0.93	2.59	3.425 (3)	150
O3—H3...O4 ⁱⁱ	0.82	1.85	2.666 (2)	176
N1—H1...O2 ⁱⁱⁱ	0.86	2.30	3.128 (2)	162
C5—H5...O4 ^{iv}	0.93	2.53	3.256 (4)	135
C10—H10...O1 ^v	0.93	2.51	3.165 (3)	127

Symmetry codes: (i) $x, -y+3/2, z-1/2$; (ii) $-x+1, -y+1, -z+2$; (iii) $x, -y+3/2, z+1/2$; (iv) $-x+1, -y+1, -z+1$; (v) $x+1, y, z$.