

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N-(2-[[5-Bromo-2-(morpholin-4-yl)-pyrimidin-4-yl]sulfonyl]-4-methoxyphenyl)-4-chlorobenzenesulfonamide

Mohan Kumar,^a L. Mallesha,^b M. A. Sridhar,^{a*} Kamini Kapoor,^c Vivek K. Gupta^c and Rajni Kant^c

^aDepartment of Studies in Physics, Manasagangotri, University of Mysore, Mysore 570 006, India, ^bPG Department of Studies in Chemistry, JSS College of Arts, Commerce and Science, Ooty Road, Mysore 570 025, India, and ^cX-ray Crystallography Laboratory, Post-Graduate Department of Physics & Electronics, University of Jammu, Jammu Tawi 180 006, India
Correspondence e-mail: mas@physics.uni-mysore.ac.in

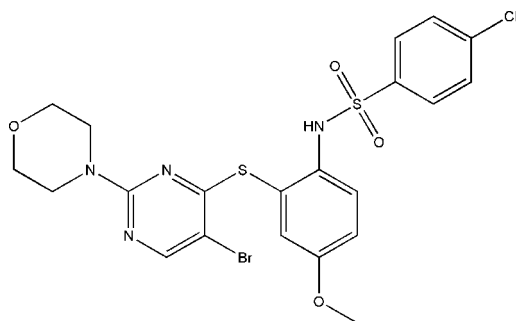
Received 22 August 2012; accepted 23 August 2012

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.045; wR factor = 0.117; data-to-parameter ratio = 15.9.

In the title compound, $\text{C}_{21}\text{H}_{20}\text{BrClN}_4\text{O}_4\text{S}_2$, the benzene rings bridged by the sulfonamide group are tilted relative to each other by a dihedral angle of $70.2(1)^\circ$ and the dihedral angle between the sulfur-bridged pyrimidine and benzene rings is $69.5(1)^\circ$. The molecular conformation is stabilized by a weak intramolecular π - π stacking interaction between the pyrimidine and the 4-chlorobenzene rings [centroid-centroid distance = $3.978(2)$ Å]. The morpholine ring adopts a chair conformation. In the crystal, molecules are linked into inversion dimers by pairs of $\text{C}-\text{H}\cdots\text{N}$ hydrogen bonds and these dimers are further connected by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a tape along the a axis.

Related literature

For related structures of sulfonamides, see: Rodrigues *et al.* (2011); Akkurt *et al.* (2011); Kant *et al.* (2012). For bond-length data, see: Allen *et al.* (1987). For ring conformations, see: Duax & Norton (1975).



Experimental

Crystal data

$\text{C}_{21}\text{H}_{20}\text{BrClN}_4\text{O}_4\text{S}_2$
 $M_r = 571.89$
Monoclinic, $P2_1/n$
 $a = 10.0311(3)$ Å
 $b = 17.3096(6)$ Å
 $c = 13.9223(4)$ Å
 $\beta = 91.829(3)^\circ$

$V = 2416.16(13)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 2.02$ mm⁻¹
 $T = 293$ K
 $0.3 \times 0.2 \times 0.2$ mm

Data collection

Oxford Diffraction Xcalibur Sapphire3 diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)
 $T_{\min} = 0.438$, $T_{\max} = 0.668$

26979 measured reflections
4744 independent reflections
3408 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.117$
 $S = 1.03$
4744 reflections

299 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.42$ e Å⁻³
 $\Delta\rho_{\min} = -0.65$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N7}-\text{H7}\cdots\text{O25}^i$	0.86	2.09	2.849 (4)	148
$\text{C20}-\text{H20}\cdots\text{N19}^{ii}$	0.93	2.52	3.352 (5)	149

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

MK acknowledges the help of Bahubali College of Engineering for his research work. RK acknowledges the Department of Science & Technology for the single-crystal X-ray diffractometer sanctioned as a National Facility under project No. SR/S2/CMP-47/2003.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS5183).

References

- Akkurt, M., Mariam, I., Naseer, I., Khan, I. U. & Sharif, S. (2011). *Acta Cryst.* **E67**, o186.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Duax, W. L. & Norton, D. A. (1975). *Atlas of Steroid Structures*, Vol. 1, New York: Plenum Press.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kant, R., Gupta, V. K., Kapoor, K., Kumar, M., Mallesha, L. & Sridhar, M. A. (2012). *Acta Cryst.* **E68**, o2590–o2591.
Oxford Diffraction (2010). *CrysAlis PRO* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
Rodrigues, V. Z., Foro, S. & Gowda, B. T. (2011). *Acta Cryst.* **E67**, o2891.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supplementary materials

Acta Cryst. (2012). E68, o2800 [doi:10.1107/S1600536812036689]

***N*-(2-[[5-Bromo-2-(morpholin-4-yl)pyrimidin-4-yl]sulfonyl]-4-methoxyphenyl)-4-chlorobenzenesulfonamide**

Mohan Kumar, L. Mallesha, M. A. Sridhar, Kamini Kapoor, Vivek K. Gupta and Rajni Kant

Comment

Bond lengths and angles in the title compound (Fig. 1) have normal values (Allen *et al.*, 1987) and are comparable with the similar crystal structures (Rodrigues *et al.*, 2011; Akkurt *et al.*, 2011; Kant *et al.*, 2012). The molecule is twisted at atom S1 with a C1—S1—N7—C8 torsion angle of 60.8 (3)°. The morpholine ring is exhibiting a chair conformation [asymmetry parameters are: $\Delta C2(N22—C23) = 2.53$; $\Delta C_s(N22—O25) = 1/5$; Duax & Norton, 1975]. The two benzene rings (C1—C6/C8—C13) are tilted relative to each other by 70.2 (1)° and the dihedral angle between the sulfur bridged pyrimidine and benzene rings is 69.5 (1)°. The molecular conformation is stabilized by a weak intramolecular stacking interaction between the pyrimidine and the 4-chloro benzene rings [centroid—centroid distance = 3.978 (2) Å, interplanar spacing = 3.340 Å, and centroid shift = 2.16 Å]. In the crystal, molecules are linked into dimers by pairs of C20—H20···N19 hydrogen bonds and these dimers are further linked by N7—H7···O25 hydrogen bonds (Table 1 and Fig. 2).

Experimental

The reaction of *N*-[2-(5-bromo-2-chloro-pyrimidin-4-ylsulfonyl)-4-methoxy-phenyl]-4-chloro-benzenesulfonamide (5.22 g, 0.01 mol) with morpholine (0.88 g, 0.01) were carried out in the presence of triethylamine and the reaction mixture was allowed to stir at room temperature for 6–7 h in dry dichloromethane. The progress of the reaction was monitored by TLC. Upon completion, the solvent was removed under reduced pressure and residue was extracted with ethyl acetate. The compound was purified by successive recrystallization from methanol (yield 80%, m.p. 462–464 K)

Refinement

All H atoms were positioned geometrically and were treated as riding on their parent C and N atoms, with C—H distances of 0.93–0.97 Å and N—H distance of 0.86 Å, and with $U_{iso}(H) = 1.2U_{eq}(C, N)$ or $1.5U_{eq}(\text{methyl C})$.

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2010); data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

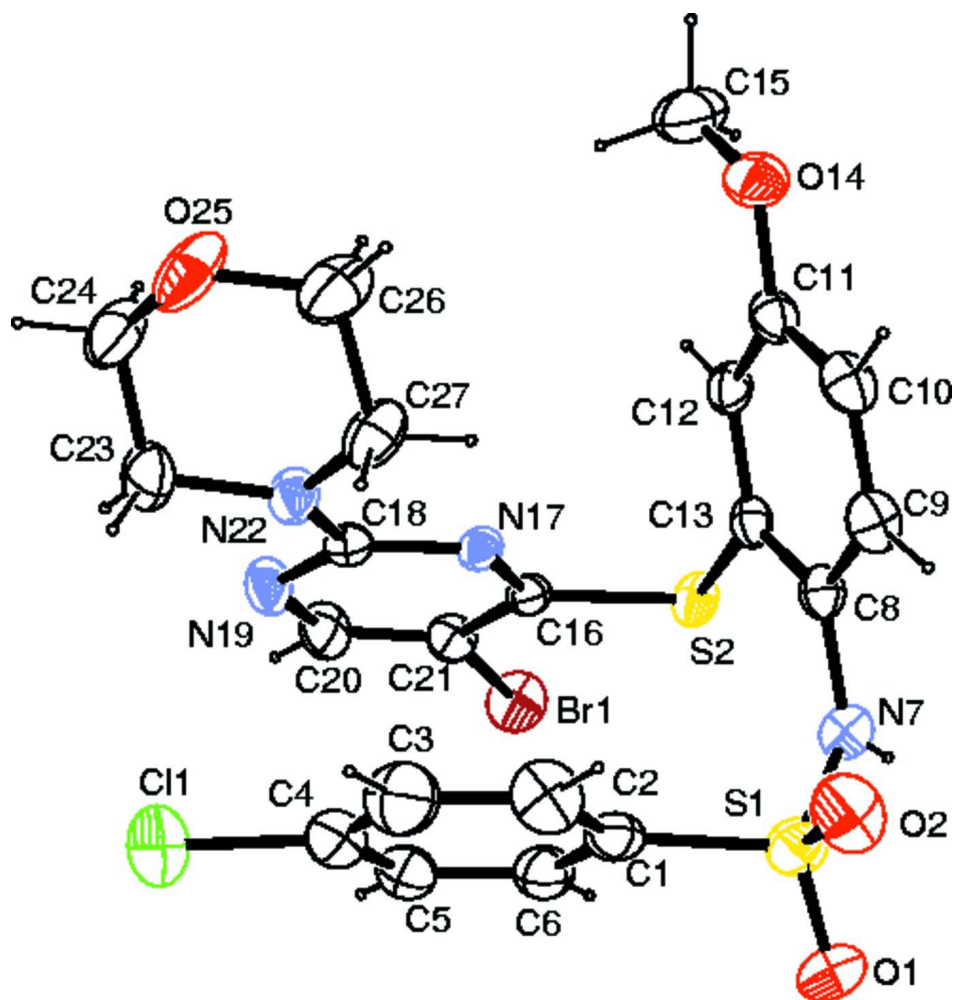


Figure 1

ORTEP view of the title molecule with the atom-labeling scheme. The displacement ellipsoids are drawn at the 40% probability level. H atoms are shown as small spheres of arbitrary radii.

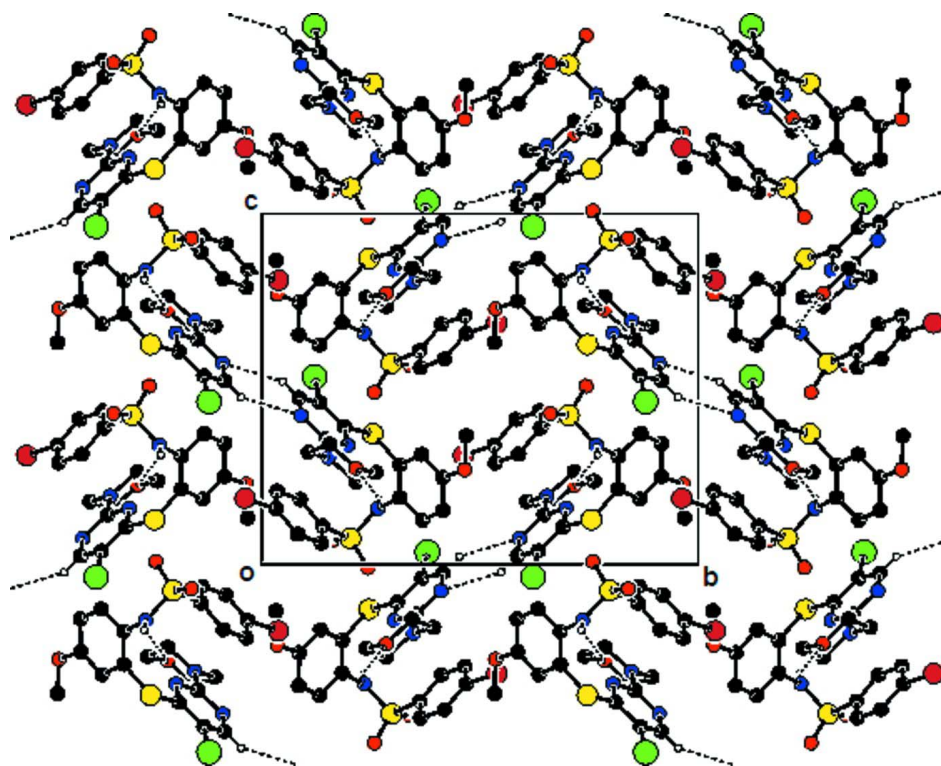


Figure 2

A molecular packing view of the title compound down the *a* axis, showing intermolecular interactions. For clarity, hydrogen atoms which are not involved in hydrogen bonding have been omitted.

***N*-(2-[[5-Bromo-2-(morpholin-4-yl)pyrimidin-4-yl]sulfonyl]-4-methoxyphenyl)-4-chlorobenzenesulfonamide**

Crystal data

$C_{21}H_{20}BrClN_4O_4S_2$

$M_r = 571.89$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 10.0311 (3) \text{ \AA}$

$b = 17.3096 (6) \text{ \AA}$

$c = 13.9223 (4) \text{ \AA}$

$\beta = 91.829 (3)^\circ$

$V = 2416.16 (13) \text{ \AA}^3$

$Z = 4$

$F(000) = 1160$

$D_x = 1.572 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9194 reflections

$\theta = 3.5\text{--}29.0^\circ$

$\mu = 2.02 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, white

$0.3 \times 0.2 \times 0.2 \text{ mm}$

Data collection

Oxford Diffraction Xcalibur Sapphire3
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 16.1049 pixels mm^{-1}

w scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2010)

$T_{\min} = 0.438$, $T_{\max} = 0.668$

26979 measured reflections

4744 independent reflections

3408 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 3.7^\circ$

$h = -12 \rightarrow 12$

$k = -21 \rightarrow 21$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.117$	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 1.7709P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
4744 reflections	$(\Delta/\sigma)_{\max} = 0.001$
299 parameters	$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. Absorption correction: *CrysAlis PRO*, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27–08-2010 CrysAlis171. NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.5036 (3)	0.16095 (19)	0.0690 (2)	0.0825 (9)
O2	0.6714 (4)	0.24236 (18)	−0.00871 (19)	0.0816 (9)
Br1	0.66487 (4)	0.12100 (3)	0.53546 (3)	0.06449 (16)
S2	0.69475 (8)	0.25466 (5)	0.37229 (6)	0.0451 (2)
S1	0.62576 (11)	0.20307 (6)	0.07413 (7)	0.0605 (3)
Cl1	1.06308 (15)	−0.03829 (9)	0.18890 (14)	0.1136 (5)
C1	0.7553 (4)	0.1383 (2)	0.1103 (3)	0.0516 (9)
C2	0.8716 (5)	0.1366 (3)	0.0617 (3)	0.0750 (12)
H2	0.8858	0.1717	0.0125	0.090*
C3	0.9679 (5)	0.0824 (3)	0.0860 (4)	0.0851 (14)
H3	1.0470	0.0803	0.0531	0.102*
C4	0.9451 (4)	0.0318 (3)	0.1593 (4)	0.0711 (12)
C5	0.8317 (4)	0.0349 (2)	0.2101 (3)	0.0647 (11)
H5	0.8197	0.0012	0.2611	0.078*
C6	0.7347 (4)	0.0882 (2)	0.1854 (3)	0.0582 (10)
H6	0.6561	0.0903	0.2190	0.070*
N7	0.6095 (3)	0.26564 (17)	0.1598 (2)	0.0492 (7)
H7	0.5343	0.2686	0.1876	0.059*
C8	0.7152 (3)	0.31610 (19)	0.1908 (2)	0.0405 (7)
C9	0.7703 (4)	0.3677 (2)	0.1266 (3)	0.0503 (9)
H9	0.7367	0.3699	0.0636	0.060*
C10	0.8737 (4)	0.4154 (2)	0.1548 (3)	0.0509 (9)
H10	0.9106	0.4487	0.1105	0.061*

C11	0.9235 (3)	0.41437 (19)	0.2487 (3)	0.0461 (8)
C12	0.8665 (3)	0.36557 (19)	0.3139 (2)	0.0431 (8)
H12	0.8964	0.3659	0.3779	0.052*
C13	0.7647 (3)	0.31593 (18)	0.2847 (2)	0.0382 (7)
O14	1.0244 (3)	0.46473 (15)	0.2706 (2)	0.0633 (7)
C15	1.0716 (5)	0.4676 (3)	0.3673 (4)	0.0833 (14)
H15A	0.9983	0.4774	0.4083	0.125*
H15B	1.1362	0.5083	0.3748	0.125*
H15C	1.1123	0.4191	0.3845	0.125*
C16	0.8284 (3)	0.18979 (17)	0.3927 (2)	0.0365 (7)
N17	0.9356 (2)	0.19637 (14)	0.33991 (18)	0.0367 (6)
C18	1.0363 (3)	0.14619 (18)	0.3584 (2)	0.0412 (8)
N19	1.0348 (3)	0.08998 (17)	0.4253 (2)	0.0555 (8)
C20	0.9257 (4)	0.0853 (2)	0.4755 (3)	0.0574 (10)
H20	0.9215	0.0474	0.5227	0.069*
C21	0.8188 (3)	0.13305 (19)	0.4616 (2)	0.0424 (8)
N22	1.1446 (3)	0.15306 (17)	0.3042 (2)	0.0521 (7)
C23	1.2648 (4)	0.1067 (3)	0.3206 (4)	0.0713 (12)
H23A	1.2512	0.0708	0.3729	0.086*
H23B	1.2824	0.0769	0.2634	0.086*
C24	1.3790 (4)	0.1560 (3)	0.3443 (4)	0.0766 (13)
H24A	1.3669	0.1796	0.4066	0.092*
H24B	1.4591	0.1246	0.3486	0.092*
O25	1.3958 (3)	0.2151 (2)	0.2743 (2)	0.0899 (11)
C26	1.2790 (4)	0.2613 (3)	0.2621 (4)	0.0846 (15)
H26A	1.2934	0.2995	0.2125	0.101*
H26B	1.2632	0.2886	0.3215	0.101*
C27	1.1609 (4)	0.2154 (3)	0.2354 (3)	0.0649 (11)
H27A	1.0824	0.2482	0.2343	0.078*
H27B	1.1704	0.1940	0.1716	0.078*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0727 (19)	0.083 (2)	0.089 (2)	-0.0082 (16)	-0.0313 (16)	-0.0141 (18)
O2	0.127 (3)	0.079 (2)	0.0388 (15)	0.0099 (19)	-0.0027 (15)	0.0047 (14)
Br1	0.0599 (3)	0.0763 (3)	0.0583 (3)	-0.0100 (2)	0.01681 (19)	0.0202 (2)
S2	0.0322 (4)	0.0552 (5)	0.0482 (5)	0.0007 (4)	0.0061 (3)	0.0165 (4)
S1	0.0729 (7)	0.0615 (6)	0.0461 (5)	-0.0010 (5)	-0.0126 (5)	-0.0021 (5)
Cl1	0.0878 (9)	0.0894 (10)	0.1623 (15)	0.0286 (8)	-0.0144 (9)	-0.0113 (9)
C1	0.058 (2)	0.049 (2)	0.048 (2)	-0.0077 (17)	-0.0057 (17)	-0.0081 (17)
C2	0.082 (3)	0.076 (3)	0.068 (3)	-0.001 (3)	0.018 (2)	0.006 (2)
C3	0.069 (3)	0.091 (4)	0.096 (4)	0.000 (3)	0.018 (3)	-0.014 (3)
C4	0.064 (3)	0.058 (3)	0.091 (3)	0.003 (2)	-0.006 (2)	-0.014 (2)
C5	0.064 (3)	0.048 (2)	0.082 (3)	-0.010 (2)	-0.007 (2)	0.005 (2)
C6	0.057 (2)	0.054 (2)	0.063 (2)	-0.0094 (19)	-0.0005 (19)	0.001 (2)
N7	0.0450 (16)	0.0564 (18)	0.0462 (16)	-0.0007 (14)	-0.0001 (13)	0.0004 (14)
C8	0.0393 (17)	0.0421 (19)	0.0405 (18)	0.0066 (14)	0.0061 (14)	0.0035 (14)
C9	0.063 (2)	0.052 (2)	0.0365 (18)	0.0063 (18)	0.0070 (16)	0.0057 (16)
C10	0.057 (2)	0.045 (2)	0.052 (2)	0.0012 (17)	0.0192 (17)	0.0131 (17)

C11	0.0397 (18)	0.0387 (19)	0.060 (2)	0.0016 (15)	0.0103 (16)	0.0091 (16)
C12	0.0398 (17)	0.044 (2)	0.0454 (19)	0.0028 (15)	-0.0019 (15)	0.0102 (15)
C13	0.0346 (16)	0.0376 (17)	0.0426 (18)	0.0048 (13)	0.0061 (14)	0.0103 (14)
O14	0.0573 (15)	0.0597 (16)	0.0730 (19)	-0.0169 (13)	0.0053 (14)	0.0132 (14)
C15	0.073 (3)	0.086 (3)	0.089 (3)	-0.032 (3)	-0.016 (3)	0.017 (3)
C16	0.0339 (16)	0.0369 (17)	0.0384 (17)	-0.0049 (13)	-0.0027 (13)	0.0033 (14)
N17	0.0300 (13)	0.0380 (15)	0.0420 (15)	-0.0040 (11)	-0.0004 (11)	0.0057 (12)
C18	0.0352 (17)	0.0381 (18)	0.050 (2)	-0.0063 (14)	-0.0007 (15)	0.0013 (15)
N19	0.0500 (17)	0.0424 (17)	0.074 (2)	0.0040 (14)	0.0052 (16)	0.0190 (15)
C20	0.060 (2)	0.047 (2)	0.065 (2)	-0.0005 (18)	0.0028 (19)	0.0229 (19)
C21	0.0440 (18)	0.0411 (19)	0.0425 (19)	-0.0075 (15)	0.0064 (15)	0.0137 (15)
N22	0.0364 (15)	0.0505 (18)	0.070 (2)	0.0009 (13)	0.0085 (14)	0.0098 (16)
C23	0.048 (2)	0.067 (3)	0.099 (3)	0.015 (2)	0.013 (2)	0.000 (2)
C24	0.042 (2)	0.092 (3)	0.095 (3)	-0.005 (2)	-0.006 (2)	0.032 (3)
O25	0.0371 (14)	0.136 (3)	0.096 (2)	-0.0163 (16)	-0.0023 (14)	0.056 (2)
C26	0.064 (3)	0.101 (4)	0.088 (3)	-0.025 (3)	-0.010 (2)	0.043 (3)
C27	0.040 (2)	0.095 (3)	0.060 (2)	-0.003 (2)	0.0070 (17)	0.017 (2)

Geometric parameters (Å, °)

O1—S1	1.426 (3)	C12—C13	1.386 (4)
O2—S1	1.427 (3)	C12—H12	0.9300
Br1—C21	1.894 (3)	O14—C15	1.414 (5)
S2—C16	1.765 (3)	C15—H15A	0.9600
S2—C13	1.777 (3)	C15—H15B	0.9600
S1—N7	1.623 (3)	C15—H15C	0.9600
S1—C1	1.777 (4)	C16—N17	1.326 (4)
C11—C4	1.736 (5)	C16—C21	1.379 (4)
C1—C2	1.367 (6)	N17—C18	1.351 (4)
C1—C6	1.379 (5)	C18—N19	1.347 (4)
C2—C3	1.381 (7)	C18—N22	1.348 (4)
C2—H2	0.9300	N19—C20	1.320 (5)
C3—C4	1.368 (7)	C20—C21	1.363 (5)
C3—H3	0.9300	C20—H20	0.9300
C4—C5	1.360 (6)	N22—C27	1.455 (5)
C5—C6	1.376 (6)	N22—C23	1.461 (5)
C5—H5	0.9300	C23—C24	1.458 (6)
C6—H6	0.9300	C23—H23A	0.9700
N7—C8	1.430 (4)	C23—H23B	0.9700
N7—H7	0.8600	C24—O25	1.426 (5)
C8—C13	1.384 (4)	C24—H24A	0.9700
C8—C9	1.391 (5)	C24—H24B	0.9700
C9—C10	1.374 (5)	O25—C26	1.424 (5)
C9—H9	0.9300	C26—C27	1.465 (6)
C10—C11	1.384 (5)	C26—H26A	0.9700
C10—H10	0.9300	C26—H26B	0.9700
C11—O14	1.363 (4)	C27—H27A	0.9700
C11—C12	1.378 (4)	C27—H27B	0.9700
C16—S2—C13	100.11 (14)	O14—C15—H15B	109.5

O1—S1—O2	120.05 (19)	H15A—C15—H15B	109.5
O1—S1—N7	105.76 (18)	O14—C15—H15C	109.5
O2—S1—N7	108.56 (17)	H15A—C15—H15C	109.5
O1—S1—C1	108.13 (18)	H15B—C15—H15C	109.5
O2—S1—C1	106.19 (19)	N17—C16—C21	121.5 (3)
N7—S1—C1	107.62 (16)	N17—C16—S2	118.8 (2)
C2—C1—C6	120.8 (4)	C21—C16—S2	119.7 (2)
C2—C1—S1	120.1 (3)	C16—N17—C18	117.0 (3)
C6—C1—S1	119.1 (3)	N19—C18—N22	118.5 (3)
C1—C2—C3	119.6 (4)	N19—C18—N17	124.9 (3)
C1—C2—H2	120.2	N22—C18—N17	116.6 (3)
C3—C2—H2	120.2	C20—N19—C18	116.0 (3)
C4—C3—C2	119.0 (4)	N19—C20—C21	123.3 (3)
C4—C3—H3	120.5	N19—C20—H20	118.3
C2—C3—H3	120.5	C21—C20—H20	118.3
C5—C4—C3	121.7 (4)	C20—C21—C16	117.3 (3)
C5—C4—C11	118.6 (4)	C20—C21—Br1	120.5 (2)
C3—C4—C11	119.7 (4)	C16—C21—Br1	122.2 (2)
C4—C5—C6	119.6 (4)	C18—N22—C27	122.9 (3)
C4—C5—H5	120.2	C18—N22—C23	122.7 (3)
C6—C5—H5	120.2	C27—N22—C23	113.7 (3)
C5—C6—C1	119.3 (4)	C24—C23—N22	110.6 (4)
C5—C6—H6	120.4	C24—C23—H23A	109.5
C1—C6—H6	120.4	N22—C23—H23A	109.5
C8—N7—S1	122.6 (2)	C24—C23—H23B	109.5
C8—N7—H7	118.7	N22—C23—H23B	109.5
S1—N7—H7	118.7	H23A—C23—H23B	108.1
C13—C8—C9	118.1 (3)	O25—C24—C23	112.0 (4)
C13—C8—N7	121.6 (3)	O25—C24—H24A	109.2
C9—C8—N7	120.3 (3)	C23—C24—H24A	109.2
C10—C9—C8	120.9 (3)	O25—C24—H24B	109.2
C10—C9—H9	119.5	C23—C24—H24B	109.2
C8—C9—H9	119.5	H24A—C24—H24B	107.9
C9—C10—C11	120.6 (3)	C26—O25—C24	111.7 (3)
C9—C10—H10	119.7	O25—C26—C27	112.4 (4)
C11—C10—H10	119.7	O25—C26—H26A	109.1
O14—C11—C12	124.5 (3)	C27—C26—H26A	109.1
O14—C11—C10	116.4 (3)	O25—C26—H26B	109.1
C12—C11—C10	119.0 (3)	C27—C26—H26B	109.1
C11—C12—C13	120.3 (3)	H26A—C26—H26B	107.8
C11—C12—H12	119.9	N22—C27—C26	110.0 (3)
C13—C12—H12	119.9	N22—C27—H27A	109.7
C8—C13—C12	121.0 (3)	C26—C27—H27A	109.7
C8—C13—S2	120.8 (2)	N22—C27—H27B	109.7
C12—C13—S2	118.1 (2)	C26—C27—H27B	109.7
C11—O14—C15	117.3 (3)	H27A—C27—H27B	108.2
O14—C15—H15A	109.5		
O1—S1—C1—C2	132.3 (3)	C11—C12—C13—S2	-179.8 (2)

O2—S1—C1—C2	2.2 (4)	C16—S2—C13—C8	111.6 (3)
N7—S1—C1—C2	-113.9 (3)	C16—S2—C13—C12	-70.9 (3)
O1—S1—C1—C6	-45.3 (3)	C12—C11—O14—C15	-1.2 (5)
O2—S1—C1—C6	-175.4 (3)	C10—C11—O14—C15	176.6 (4)
N7—S1—C1—C6	68.5 (3)	C13—S2—C16—N17	-4.3 (3)
C6—C1—C2—C3	2.1 (6)	C13—S2—C16—C21	176.6 (3)
S1—C1—C2—C3	-175.5 (4)	C21—C16—N17—C18	-1.6 (4)
C1—C2—C3—C4	-0.6 (7)	S2—C16—N17—C18	179.3 (2)
C2—C3—C4—C5	-1.6 (7)	C16—N17—C18—N19	0.8 (5)
C2—C3—C4—C11	178.4 (4)	C16—N17—C18—N22	179.7 (3)
C3—C4—C5—C6	2.4 (7)	N22—C18—N19—C20	-179.2 (3)
C11—C4—C5—C6	-177.6 (3)	N17—C18—N19—C20	-0.3 (5)
C4—C5—C6—C1	-0.9 (6)	C18—N19—C20—C21	0.6 (6)
C2—C1—C6—C5	-1.3 (6)	N19—C20—C21—C16	-1.4 (6)
S1—C1—C6—C5	176.3 (3)	N19—C20—C21—Br1	178.9 (3)
O1—S1—N7—C8	176.2 (3)	N17—C16—C21—C20	1.9 (5)
O2—S1—N7—C8	-53.7 (3)	S2—C16—C21—C20	-179.0 (3)
C1—S1—N7—C8	60.8 (3)	N17—C16—C21—Br1	-178.3 (2)
S1—N7—C8—C13	-121.0 (3)	S2—C16—C21—Br1	0.8 (4)
S1—N7—C8—C9	59.7 (4)	N19—C18—N22—C27	-175.0 (3)
C13—C8—C9—C10	2.0 (5)	N17—C18—N22—C27	6.0 (5)
N7—C8—C9—C10	-178.7 (3)	N19—C18—N22—C23	-5.6 (5)
C8—C9—C10—C11	-1.4 (5)	N17—C18—N22—C23	175.4 (3)
C9—C10—C11—O14	-178.8 (3)	C18—N22—C23—C24	-118.5 (4)
C9—C10—C11—C12	-1.0 (5)	C27—N22—C23—C24	51.7 (5)
O14—C11—C12—C13	-179.6 (3)	N22—C23—C24—O25	-53.3 (5)
C10—C11—C12—C13	2.8 (5)	C23—C24—O25—C26	56.6 (6)
C9—C8—C13—C12	-0.2 (5)	C24—O25—C26—C27	-56.8 (5)
N7—C8—C13—C12	-179.5 (3)	C18—N22—C27—C26	118.8 (4)
C9—C8—C13—S2	177.3 (2)	C23—N22—C27—C26	-51.5 (5)
N7—C8—C13—S2	-2.0 (4)	O25—C26—C27—N22	53.5 (5)
C11—C12—C13—C8	-2.2 (5)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N7—H7 \cdots O25 ⁱ	0.86	2.09	2.849 (4)	148
C20—H20 \cdots N19 ⁱⁱ	0.93	2.52	3.352 (5)	149

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