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N-(4-Chloropyridin-2-yl)-N-(4-methylphenylsulfonyl)acetamide

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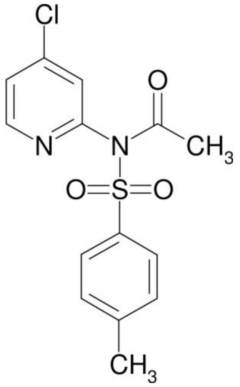
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.129; data-to-parameter ratio = 14.1.

The crystal structure of the title compound, $C_{14}H_{13}ClN_2O_3S$, features a three-dimensional network stabilized by intermolecular C—H···O hydrogen bonds between the molecules. The 4-methylphenylsulfonyl ring forms a dihedral angle of 30.6 (1)° with the 4-chloropyridine ring.

Related literature

For the biological activity of 2-alkylaminopyridinyl or 2-acylaminopyridinyl imidazole derivatives as p38α MAPK inhibitors, see: Laufer *et al.* (2008, 2010); Ziegler *et al.* (2009). For general background to protecting groups, see: Kocieński (2005). For the preparation of the *N*-protected 4-chloropyridine, see: Berliner & Belecki (2005); Sciotti *et al.* (2005); Shi & Wang (2002).



Experimental

Crystal data

$C_{14}H_{13}ClN_2O_3S$
M_r = 324.77
Orthorhombic, *Pbca*
a = 12.578 (2) Å
b = 7.5460 (8) Å
c = 30.194 (3) Å
V = 2865.7 (7) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 3.83 mm^{-1}
T = 193 K
0.35 × 0.35 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*CORINC*; Dräger & Gattow, 1971)
T_{min} = 0.872, T_{max} = 0.997
5291 measured reflections
2713 independent reflections
2412 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
3 standard reflections every 60 min intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.129
S = 1.13
2713 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O13^{i}	0.95	2.46	3.404 (3)	174
C14—H14B···O10^{ii}	0.98	2.50	3.170 (4)	126
C18—H18···O9^{iii}	0.95	2.46	3.334 (3)	152

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5410).

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supplementary materials

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N-(4-Chloropyridin-2-yl)-*N*-(4-methylphenylsulfonyl)acetamide

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Comment

In recent years, compounds with the 2-aminopyridine moiety exhibited interesting biological activities like the 2-alkylaminopyridinyl or 2-acylaminopyridinyl imidazole derivatives as p38α mitogen-activated protein kinase (p38α MAPK) inhibitors. The N-protected 4-chloropyridine is an important precursor to block the nucleophilic and basic properties of the amino-group in the C2 position of the pyridine ring. The analysis of the crystal structure shows that the aromatic C18—H-group of the 4-chloropyridine ring of one molecule interacts with the oxygen-atom O9 of the sulfonyl group of another molecule related to the first by centre of symmetry with a distance of H18···O9 2.47 Å. Furthermore, the aromatic C3—H group of the 4-methylphenylsulfonyl ring forms an intermolecular C3—H3···O13_a hydrogen bond (2.46 Å) to the oxygen atom O13 of the acetamide moiety of a third molecule. An additional hydrogen bond was observed between the methyl-group C14—H_3 of the acetamide moiety and the oxygen-atom O10 of the sulfonyl group of a further molecule, whereas the O10···H14B distance is 2.50 Å. The dihedral angle between the 4-methylphenylsulfonyl ring and the 4-chloropyridine ring is 30.6 (1)°.

Experimental

Synthesis of chloromethyl methyl ether as a solution of toluene: To a solution of dimethoxymethane (44.3 ml, 0.50 mol, 1 equiv) and $Zn(OAc)_2$ (9.2 mg, 0.01%) in toluene (133 ml) was added acetyl chloride (35.5 ml, 0.50 mol, 1 equiv). During the next 15 min, the reaction mixture warmed slowly at T = 318 K, and then cooled to ambient temperature over 3 h. The progress was again monitored until NMR analysis indicated complete conversion. The solution of MOMCl in toluene prepared using this stoichiometry is approximately 2.1 *M*.

Synthesis of *N*-(4-chloropyridin-2-yl)-4-methylbenzenesulfonamide: 2-Amino- 4-chloropyridine (20.1 g, 156 mmol. 1 equiv) and 4-toluenesulfonyl chloride (32.4 g, 168 mmol, 1.1 equiv) were dissolved in dry pyridine (70 ml) and heated at T = 353 K for 5 h. After cooling to room temperature, water was added and the compound *N*-(4-chloropyridin-2-yl)-4-methylbenzenesulfonamide dropped down as a beige solid with high analytical quality, which was filtered off and washed with water (30.6 g, 70.8%).

Synthesis of *N*-(4-chloropyridin-2-yl)-*N*-tosylacetamide: Under a nitrogen atmosphere, *N*-(4-chloropyridin-2-yl)-4-methylbenzene-sulfonamide (20.0 g, 71 mmol, 1 equiv) was added to a suspension of NaH (4.2 g, 104 mmol, 1.5 equiv) in anhydrous THF (200 ml) with stirring. The resulting reaction mixture was stirred for 20 min, and then the solution of methoxymethyl chloride in toluene (52.1 ml, 1.5 equiv) was slowly added. The mixture was stirred for 3 h and then an aqueous saturated solution of NH_4Cl was added. After separation, the aqueous layer was extracted with EtOAc, dried over Na_2SO_4 and evaporated. After treatment with hexane, the compound *N*-(4-chloropyridin-2-yl)- *N*-(methoxymethyl)-4-methylbenzenesulfonamide was obtained as the main product of the reaction (15.8 g, 69.7%) and dropped down as a pale yellow solid, whereas the compound *N*-(4-chloropyridin-2-yl)-*N*-tosylacetamide was isolated from the filtrate as the byproduct (15.4%).

Suitable crystals of the byproduct *N*-(4-chloropyridin-2-yl)-*N*-tosylacetamide for X-ray were obtained by slow evaporation at T = 298 K of a solution mixture of EtOAc/hexane.

Refinement

Hydrogen atoms were placed at calculated positions with C—H = 0.95 Å (aromatic) or 0.98–0.99 Å (sp^3 C-atom) and refined in the riding-model approximation with isotropic displacement parameters (set at 1.2–1.5 times of the U_{eq} of the parent atom).

Figures

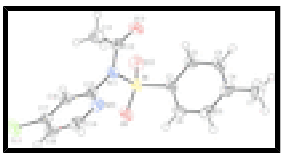


Fig. 1. View of compound **I**. Displacement ellipsoids are drawn at the 50% probability level.

N-(4-Chloropyridin-2-yl)-*N*-(4-methylphenylsulfonyl)acetamide

Crystal data

$C_{14}H_{13}ClN_2O_3S$	F(000) = 1344
M_r = 324.77	D_x = 1.506 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *K*α radiation, λ = 1.54178 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 12.578 (2) Å	θ = 65–69°
b = 7.5460 (8) Å	μ = 3.83 mm^{-1}
c = 30.194 (3) Å	*T* = 193 K
V = 2865.7 (7) Å^3	Block, colourless
Z = 8	0.35 × 0.35 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	2412 reflections with $I > 2\sigma(I)$
Radiation source: rotating anode	R_{int} = 0.079
graphite	θ_{max} = 70.0°, θ_{min} = 2.9°
ω/2θ scans	$h = -15 \rightarrow 15$
Absorption correction: ψ scan (*CORINC*; Dräger & Gattow, 1971)	$k = 0 \rightarrow 9$
T_{min} = 0.872, T_{max} = 0.997	$l = 0 \rightarrow 36$
5291 measured reflections	3 standard reflections every 60 min
2713 independent reflections	intensity decay: 2%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.0592P)^2 + 0.6955P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} = 0.001$
2713 reflections	$\Delta\rho_{max} = 0.44$ e Å^{-3}
193 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00129 (16)

Special details

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.26049 (7)	0.59127 (8)	0.519895 (18)	0.0474 (2)
C1	0.55234 (19)	0.0478 (3)	0.36074 (7)	0.0279 (5)
C2	0.5457 (2)	−0.0380 (3)	0.31992 (7)	0.0299 (5)
H2	0.4787	−0.0702	0.3079	0.036*
C3	0.6385 (2)	−0.0751 (3)	0.29725 (7)	0.0358 (6)
H3	0.6346	−0.1337	0.2694	0.043*
C4	0.7371 (2)	−0.0290 (3)	0.31410 (8)	0.0374 (6)
C5	0.7421 (2)	0.0548 (3)	0.35535 (8)	0.0379 (5)
H5	0.8093	0.0851	0.3675	0.046*
C6	0.6503 (2)	0.0940 (3)	0.37862 (7)	0.0342 (5)
H6	0.6542	0.1519	0.4065	0.041*
C7	0.8367 (3)	−0.0685 (4)	0.28847 (11)	0.0545 (8)
H7A	0.8945	−0.0963	0.3091	0.082*
H7B	0.8562	0.0351	0.2707	0.082*
H7C	0.8243	−0.1700	0.2689	0.082*
S8	0.43683 (5)	0.09319 (7)	0.390620 (16)	0.0289 (2)
O9	0.46215 (17)	0.0989 (2)	0.43669 (5)	0.0394 (4)
O10	0.35394 (15)	−0.0198 (2)	0.37556 (5)	0.0390 (4)
N11	0.40466 (17)	0.3056 (2)	0.37834 (6)	0.0295 (4)
C12	0.38183 (19)	0.3544 (3)	0.33447 (7)	0.0314 (5)

O13	0.37972 (16)	0.2443 (2)	0.30578 (5)	0.0404 (4)
C14	0.3638 (3)	0.5483 (3)	0.32551 (8)	0.0451 (6)
H14A	0.4324	0.6097	0.3245	0.068*
H14B	0.3201	0.5990	0.3492	0.068*
H14C	0.3273	0.5623	0.2971	0.068*
C15	0.41589 (19)	0.4361 (3)	0.41287 (6)	0.0270 (5)
C16	0.33884 (19)	0.4476 (3)	0.44486 (6)	0.0278 (4)
H16	0.2787	0.3713	0.4447	0.033*
C17	0.3522 (2)	0.5750 (3)	0.47748 (7)	0.0305 (5)
C18	0.4390 (2)	0.6871 (3)	0.47593 (8)	0.0373 (6)
H18	0.4488	0.7773	0.4975	0.045*
C19	0.5105 (2)	0.6634 (3)	0.44216 (8)	0.0389 (6)
H19	0.5704	0.7400	0.4411	0.047*
N20	0.50149 (17)	0.5390 (3)	0.41048 (6)	0.0343 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0655 (5)	0.0449 (4)	0.0320 (3)	0.0135 (3)	0.0132 (3)	−0.0045 (2)
C1	0.0379 (13)	0.0247 (10)	0.0211 (9)	0.0010 (9)	−0.0010 (8)	0.0012 (8)
C2	0.0408 (13)	0.0237 (10)	0.0251 (10)	−0.0023 (10)	−0.0025 (9)	−0.0026 (8)
C3	0.0527 (15)	0.0273 (10)	0.0274 (10)	0.0045 (11)	0.0038 (11)	−0.0014 (8)
C4	0.0440 (15)	0.0286 (11)	0.0396 (11)	0.0089 (11)	0.0078 (11)	0.0102 (9)
C5	0.0349 (13)	0.0353 (12)	0.0436 (12)	0.0010 (10)	−0.0063 (11)	0.0064 (10)
C6	0.0455 (15)	0.0296 (11)	0.0275 (10)	0.0013 (10)	−0.0086 (10)	−0.0012 (8)
C7	0.0509 (18)	0.0453 (15)	0.0675 (18)	0.0124 (14)	0.0187 (16)	0.0125 (13)
S8	0.0396 (4)	0.0244 (3)	0.0225 (3)	0.0014 (2)	0.0028 (2)	0.00126 (17)
O9	0.0628 (12)	0.0318 (8)	0.0236 (8)	0.0098 (8)	0.0048 (8)	0.0027 (6)
O10	0.0411 (10)	0.0320 (8)	0.0438 (9)	−0.0061 (8)	0.0062 (7)	0.0011 (7)
N11	0.0382 (11)	0.0257 (9)	0.0244 (8)	0.0029 (8)	0.0009 (7)	−0.0017 (7)
C12	0.0326 (12)	0.0350 (11)	0.0265 (10)	0.0013 (10)	−0.0022 (9)	0.0019 (9)
O13	0.0564 (11)	0.0390 (9)	0.0257 (7)	0.0014 (9)	−0.0055 (7)	−0.0002 (7)
C14	0.0530 (16)	0.0427 (14)	0.0397 (12)	0.0063 (13)	0.0026 (12)	0.0058 (11)
C15	0.0336 (11)	0.0252 (10)	0.0221 (9)	0.0050 (9)	−0.0035 (8)	0.0013 (7)
C16	0.0327 (11)	0.0256 (10)	0.0252 (9)	0.0019 (9)	−0.0014 (8)	0.0014 (8)
C17	0.0397 (13)	0.0281 (10)	0.0235 (9)	0.0091 (10)	−0.0021 (9)	0.0020 (8)
C18	0.0520 (15)	0.0272 (11)	0.0327 (11)	0.0039 (11)	−0.0129 (10)	−0.0039 (9)
C19	0.0379 (13)	0.0321 (12)	0.0467 (13)	−0.0030 (11)	−0.0089 (11)	0.0011 (10)
N20	0.0350 (11)	0.0315 (10)	0.0364 (10)	0.0005 (9)	−0.0008 (8)	0.0025 (8)

Geometric parameters (Å, °)

Cl1—C17	1.728 (2)	S8—N11	1.6942 (18)
C1—C6	1.390 (3)	N11—C12	1.405 (3)
C1—C2	1.395 (3)	N11—C15	1.441 (3)
C1—S8	1.744 (2)	C12—O13	1.201 (3)
C2—C3	1.382 (4)	C12—C14	1.505 (3)
C2—H2	0.9500	C14—H14A	0.9800
C3—C4	1.385 (4)	C14—H14B	0.9800

C3—H3	0.9500	C14—H14C	0.9800
C4—C5	1.398 (4)	C15—N20	1.329 (3)
C4—C7	1.502 (4)	C15—C16	1.371 (3)
C5—C6	1.384 (4)	C16—C17	1.387 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—H6	0.9500	C17—C18	1.381 (4)
C7—H7A	0.9800	C18—C19	1.371 (4)
C7—H7B	0.9800	C18—H18	0.9500
C7—H7C	0.9800	C19—N20	1.345 (3)
S8—O10	1.4213 (19)	C19—H19	0.9500
S8—O9	1.4276 (16)		

C6—C1—C2	120.8 (2)	N11—S8—C1	105.75 (10)
C6—C1—S8	119.24 (16)	C12—N11—C15	121.53 (18)
C2—C1—S8	119.92 (18)	C12—N11—S8	120.24 (15)
C3—C2—C1	118.8 (2)	C15—N11—S8	117.69 (14)
C3—C2—H2	120.6	O13—C12—N11	120.2 (2)
C1—C2—H2	120.6	O13—C12—C14	122.7 (2)
C2—C3—C4	121.5 (2)	N11—C12—C14	117.1 (2)
C2—C3—H3	119.2	C12—C14—H14A	109.5
C4—C3—H3	119.2	C12—C14—H14B	109.5
C3—C4—C5	118.8 (2)	H14A—C14—H14B	109.5
C3—C4—C7	120.5 (2)	C12—C14—H14C	109.5
C5—C4—C7	120.7 (3)	H14A—C14—H14C	109.5
C6—C5—C4	120.8 (2)	H14B—C14—H14C	109.5
C6—C5—H5	119.6	N20—C15—C16	125.0 (2)
C4—C5—H5	119.6	N20—C15—N11	116.06 (19)
C5—C6—C1	119.3 (2)	C16—C15—N11	118.9 (2)
C5—C6—H6	120.4	C15—C16—C17	117.3 (2)
C1—C6—H6	120.4	C15—C16—H16	121.4
C4—C7—H7A	109.5	C17—C16—H16	121.4
C4—C7—H7B	109.5	C18—C17—C16	119.8 (2)
H7A—C7—H7B	109.5	C18—C17—Cl1	120.60 (17)
C4—C7—H7C	109.5	C16—C17—Cl1	119.64 (19)
H7A—C7—H7C	109.5	C19—C18—C17	117.6 (2)
H7B—C7—H7C	109.5	C19—C18—H18	121.2
O10—S8—O9	119.57 (11)	C17—C18—H18	121.2
O10—S8—N11	108.79 (10)	N20—C19—C18	124.4 (2)
O9—S8—N11	103.77 (9)	N20—C19—H19	117.8
O10—S8—C1	109.13 (10)	C18—C19—H19	117.8
O9—S8—C1	108.91 (12)	C15—N20—C19	115.9 (2)

C6—C1—C2—C3	−0.5 (3)	O9—S8—N11—C15	3.9 (2)
S8—C1—C2—C3	−178.90 (16)	C1—S8—N11—C15	−110.65 (18)
C1—C2—C3—C4	−0.1 (3)	C15—N11—C12—O13	175.1 (2)
C2—C3—C4—C5	1.0 (3)	S8—N11—C12—O13	3.8 (3)
C2—C3—C4—C7	−179.1 (2)	C15—N11—C12—C14	−3.2 (3)
C3—C4—C5—C6	−1.2 (4)	S8—N11—C12—C14	−174.53 (19)
C7—C4—C5—C6	178.9 (2)	C12—N11—C15—N20	−69.5 (3)
C4—C5—C6—C1	0.6 (3)	S8—N11—C15—N20	102.1 (2)

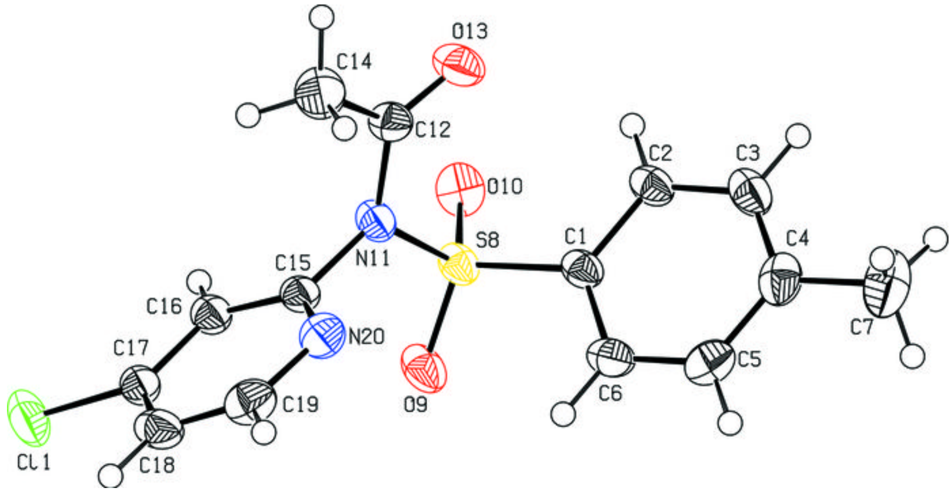
C2—C1—C6—C5	0.3 (3)	C12—N11—C15—C16	109.6 (2)
S8—C1—C6—C5	178.69 (17)	S8—N11—C15—C16	−78.8 (2)
C6—C1—S8—O10	−158.12 (17)	N20—C15—C16—C17	−0.8 (3)
C2—C1—S8—O10	20.3 (2)	N11—C15—C16—C17	−179.85 (18)
C6—C1—S8—O9	−26.0 (2)	C15—C16—C17—C18	1.9 (3)
C2—C1—S8—O9	152.42 (17)	C15—C16—C17—Cl1	−177.71 (16)
C6—C1—S8—N11	85.00 (19)	C16—C17—C18—C19	−1.6 (3)
C2—C1—S8—N11	−96.60 (19)	Cl1—C17—C18—C19	178.00 (18)
O10—S8—N11—C12	−56.1 (2)	C17—C18—C19—N20	0.2 (4)
O9—S8—N11—C12	175.60 (19)	C16—C15—N20—C19	−0.5 (3)
C1—S8—N11—C12	61.0 (2)	N11—C15—N20—C19	178.49 (19)
O10—S8—N11—C15	132.24 (18)	C18—C19—N20—C15	0.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O13^{i}	0.95	2.46	3.404 (3)	174
C14—H14B···O10^{ii}	0.98	2.50	3.170 (4)	126
C18—H18···O9^{iii}	0.95	2.46	3.334 (3)	152

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1/2, *y*+1/2, *z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Fig. 1


O13
C14
C12
C2
C3
O10
N11
S8
C1
C4
C15
C16
N20
C7
C17
C5
C6
O9
C19
Cl1
C18