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Piperidinium 4-(4-chlorophenyl)-3-cyano-5-ethoxycarbonyl-6-methylpyridine-2-thiolate

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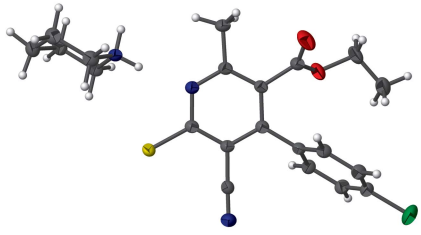
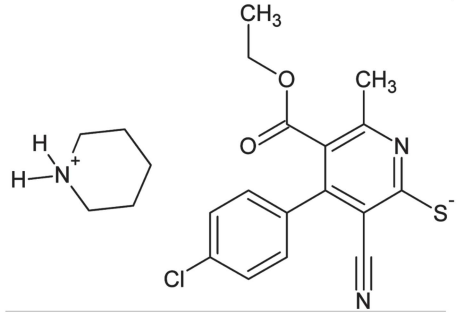
In the crystal of the title salt, $C_5H_{12}N^+\cdot C_{16}H_{12}ClN_2O_2S^-$, the cation adopts a chair conformation, and N—H···N and N—H···S hydrogen bonds form chains of alternating cations and anions running parallel to the *c* axis. The crystal structure contains a solvent-accessible void of 50 Å^3, but no solvent molecule is located there.

3D view



Chemical scheme



Structure description

Pyridine derivatives continue to attract great interest due to the wide variety of interesting biological activities observed for these compounds, such as anticancer, analgesic, antimicrobial and antidepressant activities (Kumar *et al.*, 2011). In addition, pyridines are used in the pharmaceutical industry as raw materials for the synthesis of various drugs, vitamins and fungicides (Kumar *et al.*, 2011). These facts prompted us to synthesize the title compound, which contains both pyridine and piperidine moieties, and confirm its crystal structure by X-ray analysis.

In the anion (Fig. 1), the dihedral angle between the pyridine and chlorobenze rings is 69.48 (7)°. The cation has a chair conformation with puckering parameters of Q_T = 0.5684 (16) Å, θ = 176.46 (16) and φ = 199 (3)°.

In the crystal, the cations and anions are linked by N—H···N and N—H···S hydrogen bonds (Table 1), forming chains of alternating cations and anions parallel to the *c* axis (Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···N1	0.92 (2)	2.01 (2)	2.9288 (17)	174.5 (17)
N3—H3B···S1^{i}	0.93 (2)	2.64 (2)	3.4249 (12)	142.6 (15)

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Synthesis and crystallization

The title compound was prepared by refluxing equimolar quantities of ethyl 3-cyano-1,2-dihydro-6-methyl-4-(4-chlorophenyl)-2-thioxopyridine-5-carboxylate and piperidine (10 mmol) in absolute ethanol (25 ml) for 5 min. The product that formed on cooling was collected and recrystallized from ethanol (95%) as yellow needles. Yield: 83%, m. p. 433–435 K.

IR: 3410, 2520, 2400 (N^+H_2), 2964 (C—H, aliphatic), 2217 (C≡N), 1713 (C=O) cm$^{-1.}$ ^{1}H NMR ($CDCl_3$) δ: 7.35 (*s*, 2H, N^+H_2), 7.19–7.33 (*m*, 4H, Ar—H), 3.89–3.90 (*q*, 2H, OCH_2), 3.17 (*t*, 4H, CH_2NCH_2), 2.41 (*s*, 3H, CH_3), 1.79 (*m*, 2H, CH_2), 1.61 (*m*, 2H, CH_2), 1.19–1.25 (*m*, 2H, CH_2), 0.84 (*t*, 3H, CH_3). Elemental analysis calculated for $C_{21}H_{24}ClN_3O_2S$ (%): C, 60.35; H, 5.79; N, 10.05; S, 7.67. Found (%): C, 60.28; H, 5.68; N, 10.09; S, 7.33.

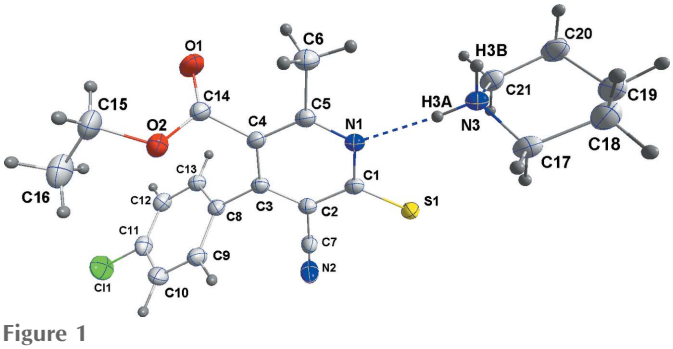


Figure 1
The title molecule with labeling scheme and 50% probability ellipsoids.

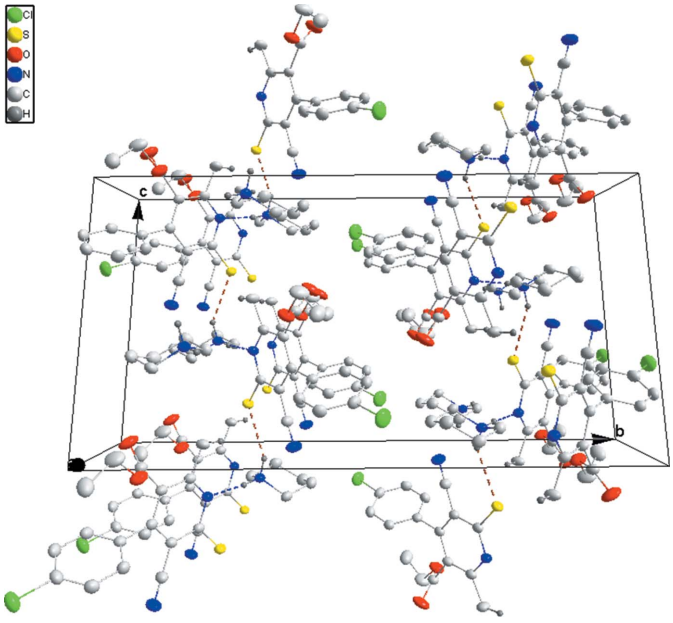


Figure 2
Packing viewed along the *a* axis with N—H···N and N—H···S hydrogen bonds shown as blue and brown dashed lines, respectively.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_5H_{12}N^+\cdot C_{16}H_{12}ClN_2O_2S^-$
M_r	417.94
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	7.2363 (2), 24.2600 (7), 12.9049 (4)
β (°)	105.603 (1)
V (Å^3)	2182.00 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	2.61
Crystal size (mm)	0.26 × 0.14 × 0.13
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.61, 0.72
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16665, 4350, 3985
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.097, 1.04
No. of reflections	4350
No. of parameters	263
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.46

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160651 [doi:10.1107/S2414314616006519]

Piperidinium 4-(4-chlorophenyl)-3-cyano-5-ethoxycarbonyl-6-methylpyridine-2-thiolate

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Piperidin-1-ium [4-(4-chlorophenyl)-3-cyano-5-(ethoxycarbonyl)-6-methylpyridin-2-yl]sulfanide

Crystal data

$C_5H_{12}N^+·C_{16}H_{12}ClN_2O_2S^-$
M_r = 417.94
Monoclinic, $P2_1/c$
a = 7.2363 (2) Å
b = 24.2600 (7) Å
c = 12.9049 (4) Å
β = 105.603 (1)°
V = 2182.00 (11) Å^3
Z = 4
$F(000)$ = 880
D_x = 1.272 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9892 reflections
θ = 3.6–74.3°
μ = 2.61 mm^{-1}
T = 150 K
Block, colourless
0.26 × 0.14 × 0.13 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro–focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.61, T_{max} = 0.72
16665 measured reflections
4350 independent reflections
3985 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 74.6°, θ_{min} = 3.6°
h = −9→8
k = −30→29
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.097
S = 1.04
4350 reflections
263 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0538P)^2 + 0.8348P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached carbon atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.39999 (7)	0.47748 (2)	0.81495 (4)	0.04801 (14)
S1	0.59234 (5)	0.72882 (2)	0.82912 (3)	0.02541 (11)
O1	−0.01709 (18)	0.59943 (6)	0.41297 (10)	0.0469 (3)
O2	−0.21430 (15)	0.63592 (5)	0.50149 (9)	0.0366 (3)
N1	0.37767 (17)	0.71321 (5)	0.62901 (9)	0.0245 (2)
N2	0.3246 (2)	0.63295 (6)	0.96028 (10)	0.0395 (3)
C1	0.4064 (2)	0.69910 (6)	0.73433 (11)	0.0226 (3)
C2	0.2804 (2)	0.66016 (6)	0.76156 (10)	0.0230 (3)
C3	0.13227 (19)	0.63537 (6)	0.68331 (10)	0.0223 (3)
C4	0.1123 (2)	0.64998 (6)	0.57583 (10)	0.0231 (3)
C5	0.2355 (2)	0.68969 (6)	0.55271 (11)	0.0246 (3)
C6	0.2084 (2)	0.71053 (7)	0.43991 (11)	0.0333 (3)
H6A	0.2103	0.6794	0.3918	0.050*
H6B	0.3123	0.7361	0.4382	0.050*
H6C	0.0849	0.7297	0.4161	0.050*
C7	0.3071 (2)	0.64525 (6)	0.87240 (11)	0.0270 (3)
C8	0.0020 (2)	0.59527 (6)	0.71526 (10)	0.0229 (3)
C9	−0.1251 (2)	0.61412 (6)	0.77162 (11)	0.0270 (3)
H9	−0.1268	0.6521	0.7891	0.032*
C10	−0.2488 (2)	0.57806 (6)	0.80233 (12)	0.0300 (3)
H10	−0.3361	0.5910	0.8401	0.036*
C11	−0.2431 (2)	0.52261 (6)	0.77703 (12)	0.0295 (3)
C12	−0.1176 (2)	0.50282 (6)	0.72201 (12)	0.0291 (3)
H12	−0.1150	0.4647	0.7057	0.035*
C13	0.0050 (2)	0.53949 (6)	0.69076 (11)	0.0261 (3)
H13	0.0914	0.5264	0.6524	0.031*
C14	−0.0433 (2)	0.62493 (6)	0.48768 (11)	0.0265 (3)
C15	−0.3827 (3)	0.61023 (9)	0.42940 (14)	0.0456 (4)
H15A	−0.3432	0.5850	0.3789	0.055*
H15B	−0.4682	0.6388	0.3870	0.055*
C16	−0.4853 (3)	0.57877 (8)	0.49676 (16)	0.0458 (4)
H16A	−0.6079	0.5652	0.4512	0.069*
H16B	−0.5090	0.6030	0.5526	0.069*
H16C	−0.4062	0.5475	0.5307	0.069*

N3	0.65498 (18)	0.79520 (5)	0.59790 (9)	0.0248 (3)
H3A	0.572 (3)	0.7694 (8)	0.6125 (15)	0.038 (5)*
H3B	0.604 (3)	0.8040 (8)	0.5259 (16)	0.036 (5)*
C17	0.6606 (2)	0.84628 (6)	0.66329 (11)	0.0286 (3)
H17A	0.7135	0.8375	0.7405	0.034*
H17B	0.5288	0.8607	0.6527	0.034*
C18	0.7836 (2)	0.88953 (6)	0.63022 (13)	0.0323 (3)
H18A	0.7904	0.9226	0.6761	0.039*
H18B	0.7241	0.9005	0.5547	0.039*
C19	0.9854 (2)	0.86807 (7)	0.64069 (13)	0.0343 (3)
H19A	1.0520	0.8624	0.7176	0.041*
H19B	1.0586	0.8957	0.6115	0.041*
C20	0.9797 (2)	0.81383 (7)	0.57999 (13)	0.0333 (3)
H20A	0.9329	0.8209	0.5017	0.040*
H20B	1.1113	0.7987	0.5947	0.040*
C21	0.8506 (2)	0.77161 (6)	0.61209 (12)	0.0299 (3)
H21A	0.8424	0.7382	0.5670	0.036*
H21B	0.9054	0.7609	0.6882	0.036*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0480 (3)	0.0416 (2)	0.0606 (3)	−0.01460 (19)	0.0251 (2)	0.00572 (19)
S1	0.02572 (18)	0.02913 (19)	0.02096 (17)	−0.00411 (13)	0.00555 (13)	−0.00248 (12)
O1	0.0394 (7)	0.0654 (9)	0.0355 (6)	−0.0050 (6)	0.0094 (5)	−0.0263 (6)
O2	0.0245 (5)	0.0521 (7)	0.0311 (5)	−0.0041 (5)	0.0038 (4)	−0.0120 (5)
N1	0.0267 (6)	0.0266 (6)	0.0211 (5)	−0.0012 (5)	0.0080 (5)	−0.0011 (4)
N2	0.0400 (8)	0.0512 (9)	0.0247 (7)	−0.0119 (7)	0.0044 (6)	0.0053 (6)
C1	0.0240 (7)	0.0237 (6)	0.0210 (6)	0.0028 (5)	0.0076 (5)	−0.0017 (5)
C2	0.0249 (7)	0.0249 (6)	0.0197 (6)	0.0011 (5)	0.0070 (5)	0.0000 (5)
C3	0.0230 (7)	0.0228 (6)	0.0219 (6)	0.0022 (5)	0.0073 (5)	−0.0017 (5)
C4	0.0241 (7)	0.0256 (6)	0.0194 (6)	0.0007 (5)	0.0056 (5)	−0.0029 (5)
C5	0.0265 (7)	0.0274 (7)	0.0206 (6)	0.0008 (6)	0.0073 (5)	−0.0015 (5)
C6	0.0392 (9)	0.0400 (8)	0.0206 (7)	−0.0076 (7)	0.0079 (6)	0.0014 (6)
C7	0.0257 (7)	0.0302 (7)	0.0240 (7)	−0.0046 (6)	0.0049 (5)	−0.0006 (6)
C8	0.0236 (7)	0.0255 (6)	0.0189 (6)	−0.0001 (5)	0.0043 (5)	0.0004 (5)
C9	0.0300 (7)	0.0253 (7)	0.0275 (7)	−0.0014 (6)	0.0107 (6)	−0.0037 (5)
C10	0.0297 (7)	0.0341 (8)	0.0292 (7)	−0.0012 (6)	0.0131 (6)	−0.0017 (6)
C11	0.0290 (7)	0.0300 (7)	0.0288 (7)	−0.0053 (6)	0.0066 (6)	0.0045 (6)
C12	0.0336 (8)	0.0225 (6)	0.0296 (7)	−0.0002 (6)	0.0057 (6)	0.0011 (5)
C13	0.0277 (7)	0.0264 (7)	0.0245 (6)	0.0020 (6)	0.0074 (5)	−0.0005 (5)
C14	0.0292 (7)	0.0290 (7)	0.0209 (6)	−0.0022 (6)	0.0059 (5)	−0.0013 (5)
C15	0.0298 (8)	0.0668 (12)	0.0345 (8)	−0.0117 (8)	−0.0014 (7)	−0.0086 (8)
C16	0.0367 (9)	0.0450 (10)	0.0478 (10)	−0.0083 (8)	−0.0021 (8)	0.0044 (8)
N3	0.0275 (6)	0.0272 (6)	0.0200 (5)	−0.0009 (5)	0.0069 (5)	−0.0001 (5)
C17	0.0329 (8)	0.0297 (7)	0.0233 (6)	0.0028 (6)	0.0078 (6)	−0.0046 (5)
C18	0.0369 (8)	0.0273 (7)	0.0306 (7)	−0.0002 (6)	0.0058 (6)	−0.0031 (6)
C19	0.0333 (8)	0.0364 (8)	0.0322 (8)	−0.0066 (7)	0.0069 (6)	−0.0037 (6)

C20	0.0292 (8)	0.0393 (8)	0.0332 (8)	−0.0001 (7)	0.0113 (6)	−0.0062 (6)
C21	0.0306 (8)	0.0291 (7)	0.0295 (7)	0.0044 (6)	0.0070 (6)	−0.0023 (6)

Geometric parameters (Å, º)

Cl1—C11	1.7398 (15)	C12—H12	0.9500
S1—C1	1.7150 (14)	C13—H13	0.9500
O1—C14	1.2027 (18)	C15—C16	1.496 (3)
O2—C14	1.3238 (19)	C15—H15A	0.9900
O2—C15	1.4591 (19)	C15—H15B	0.9900
N1—C5	1.3447 (18)	C16—H16A	0.9800
N1—C1	1.3623 (17)	C16—H16B	0.9800
N2—C7	1.146 (2)	C16—H16C	0.9800
C1—C2	1.4212 (19)	N3—C21	1.4918 (19)
C2—C3	1.3957 (19)	N3—C17	1.4937 (18)
C2—C7	1.4371 (19)	N3—H3A	0.92 (2)
C3—C4	1.4009 (18)	N3—H3B	0.93 (2)
C3—C8	1.4877 (19)	C17—C18	1.510 (2)
C4—C5	1.399 (2)	C17—H17A	0.9900
C4—C14	1.4973 (19)	C17—H17B	0.9900
C5—C6	1.5031 (19)	C18—C19	1.522 (2)
C6—H6A	0.9800	C18—H18A	0.9900
C6—H6B	0.9800	C18—H18B	0.9900
C6—H6C	0.9800	C19—C20	1.526 (2)
C8—C13	1.3912 (19)	C19—H19A	0.9900
C8—C9	1.3945 (19)	C19—H19B	0.9900
C9—C10	1.383 (2)	C20—C21	1.517 (2)
C9—H9	0.9500	C20—H20A	0.9900
C10—C11	1.387 (2)	C20—H20B	0.9900
C10—H10	0.9500	C21—H21A	0.9900
C11—C12	1.381 (2)	C21—H21B	0.9900
C12—C13	1.391 (2)		

C14—O2—C15	118.59 (13)	C16—C15—H15A	110.1
C5—N1—C1	120.36 (12)	O2—C15—H15B	110.1
N1—C1—C2	118.54 (12)	C16—C15—H15B	110.1
N1—C1—S1	119.07 (10)	H15A—C15—H15B	108.4
C2—C1—S1	122.38 (10)	C15—C16—H16A	109.5
C3—C2—C1	121.77 (12)	C15—C16—H16B	109.5
C3—C2—C7	118.90 (13)	H16A—C16—H16B	109.5
C1—C2—C7	119.32 (12)	C15—C16—H16C	109.5
C2—C3—C4	117.52 (13)	H16A—C16—H16C	109.5
C2—C3—C8	120.11 (12)	H16B—C16—H16C	109.5
C4—C3—C8	122.37 (12)	C21—N3—C17	111.59 (11)
C5—C4—C3	118.92 (12)	C21—N3—H3A	111.3 (12)
C5—C4—C14	120.65 (12)	C17—N3—H3A	111.6 (12)
C3—C4—C14	120.39 (12)	C21—N3—H3B	108.7 (12)
N1—C5—C4	122.83 (12)	C17—N3—H3B	108.5 (12)

N1—C5—C6	116.19 (13)	H3A—N3—H3B	104.8 (17)
C4—C5—C6	120.91 (13)	N3—C17—C18	110.21 (12)
C5—C6—H6A	109.5	N3—C17—H17A	109.6
C5—C6—H6B	109.5	C18—C17—H17A	109.6
H6A—C6—H6B	109.5	N3—C17—H17B	109.6
C5—C6—H6C	109.5	C18—C17—H17B	109.6
H6A—C6—H6C	109.5	H17A—C17—H17B	108.1
H6B—C6—H6C	109.5	C17—C18—C19	111.20 (13)
N2—C7—C2	178.55 (16)	C17—C18—H18A	109.4
C13—C8—C9	119.36 (13)	C19—C18—H18A	109.4
C13—C8—C3	121.55 (12)	C17—C18—H18B	109.4
C9—C8—C3	119.09 (12)	C19—C18—H18B	109.4
C10—C9—C8	120.70 (14)	H18A—C18—H18B	108.0
C10—C9—H9	119.7	C18—C19—C20	110.88 (13)
C8—C9—H9	119.7	C18—C19—H19A	109.5
C9—C10—C11	118.89 (14)	C20—C19—H19A	109.5
C9—C10—H10	120.6	C18—C19—H19B	109.5
C11—C10—H10	120.6	C20—C19—H19B	109.5
C12—C11—C10	121.56 (14)	H19A—C19—H19B	108.1
C12—C11—Cl1	119.68 (12)	C21—C20—C19	112.07 (13)
C10—C11—Cl1	118.76 (12)	C21—C20—H20A	109.2
C11—C12—C13	119.07 (14)	C19—C20—H20A	109.2
C11—C12—H12	120.5	C21—C20—H20B	109.2
C13—C12—H12	120.5	C19—C20—H20B	109.2
C12—C13—C8	120.41 (13)	H20A—C20—H20B	107.9
C12—C13—H13	119.8	N3—C21—C20	109.95 (12)
C8—C13—H13	119.8	N3—C21—H21A	109.7
O1—C14—O2	124.49 (14)	C20—C21—H21A	109.7
O1—C14—C4	124.71 (14)	N3—C21—H21B	109.7
O2—C14—C4	110.78 (12)	C20—C21—H21B	109.7
O2—C15—C16	107.90 (14)	H21A—C21—H21B	108.2
O2—C15—H15A	110.1		

C5—N1—C1—C2	−1.5 (2)	C13—C8—C9—C10	−0.6 (2)
C5—N1—C1—S1	178.60 (10)	C3—C8—C9—C10	179.78 (13)
N1—C1—C2—C3	1.5 (2)	C8—C9—C10—C11	0.6 (2)
S1—C1—C2—C3	−178.53 (11)	C9—C10—C11—C12	−0.1 (2)
N1—C1—C2—C7	−179.30 (13)	C9—C10—C11—Cl1	−179.55 (12)
S1—C1—C2—C7	0.63 (19)	C10—C11—C12—C13	−0.4 (2)
C1—C2—C3—C4	0.4 (2)	Cl1—C11—C12—C13	179.03 (11)
C7—C2—C3—C4	−178.80 (13)	C11—C12—C13—C8	0.4 (2)
C1—C2—C3—C8	−179.31 (12)	C9—C8—C13—C12	0.1 (2)
C7—C2—C3—C8	1.5 (2)	C3—C8—C13—C12	179.68 (13)
C2—C3—C4—C5	−2.29 (19)	C15—O2—C14—O1	7.8 (2)
C8—C3—C4—C5	177.38 (12)	C15—O2—C14—C4	−173.92 (14)
C2—C3—C4—C14	179.91 (12)	C5—C4—C14—O1	59.9 (2)
C8—C3—C4—C14	−0.4 (2)	C3—C4—C14—O1	−122.30 (17)
C1—N1—C5—C4	−0.5 (2)	C5—C4—C14—O2	−118.34 (15)

C1—N1—C5—C6	176.48 (13)	C3—C4—C14—O2	59.42 (18)
C3—C4—C5—N1	2.5 (2)	C14—O2—C15—C16	123.12 (17)
C14—C4—C5—N1	−179.73 (13)	C21—N3—C17—C18	59.88 (15)
C3—C4—C5—C6	−174.38 (13)	N3—C17—C18—C19	−56.81 (16)
C14—C4—C5—C6	3.4 (2)	C17—C18—C19—C20	53.36 (17)
C2—C3—C8—C13	−111.09 (15)	C18—C19—C20—C21	−52.65 (18)
C4—C3—C8—C13	69.24 (18)	C17—N3—C21—C20	−58.50 (15)
C2—C3—C8—C9	68.53 (18)	C19—C20—C21—N3	54.82 (17)
C4—C3—C8—C9	−111.14 (15)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···N1	0.92 (2)	2.01 (2)	2.9288 (17)	174.5 (17)
N3—H3*B*···S1^{i}	0.93 (2)	2.64 (2)	3.4249 (12)	142.6 (15)

Symmetry code: (i) x, $-y+3/2$, $z-1/2$.