Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-{1-[(2-Chlorothiazol-5-yl)methyl]-2-[(2-chlorothiazol-5-yl)methylsulfanyl]-4-methyl-6-phenyl-1,6-dihydropyrimidin-5-yl}ethanone

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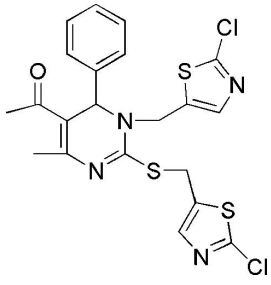
Received 11 April 2007; accepted 10 July 2007

Key indicators: single-crystal X-ray study; T = 300 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.134; data-to-parameter ratio = 17.5.

The crystal structure of the title compound, $C_{21}H_{18}Cl_2N_4OS_3$, is stabilized by intermolecular C—H···O and C—H···N hydrogen bonds. The dihydropyrimidine ring is almost planer, with a mean deviation from the plane of 0.132 (1) Å. The dihedral angles between the dihydropyrimidine ring and the phenyl, 1-thiazole and 2-thiazole rings are 88.5 (1), 13.6 (1) and 8.0 (1)°, respectively.

Related literature

For general background, see: Kappe (1993).



Experimental

Crystal data

$C_{21}H_{18}Cl_2N_4OS_3$
M_r = 509.47
Monoclinic, $P2_1/c$
a = 10.6123 (5) Å
b = 18.7414 (6) Å
c = 12.4631 (9) Å
β = 113.820 (1)°
V = 2267.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.59 mm^{-1}
T = 300 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.844, T_{max} = 0.892
15492 measured reflections
4937 independent reflections
3980 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.134
S = 1.07
4937 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18A···N1	0.97	2.39	2.799 (3)	105
C14—H14A···S2	0.97	2.51	2.972 (2)	109
C7—H7···O1	0.98	2.32	2.687 (3)	101
C18—H18B···O1^{i}	0.97	2.39	3.314 (3)	159
C12—H12A···N3^{ii}	0.96	2.45	3.390 (3)	167

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Natural Science Foundation of China (grant No. 20302002) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2011).

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  doi:10.1107/S1600536807033764

supplementary materials

Acta Cryst. (2007). E**63**, o3516 [**doi:10.1107/S1600536807033764**]

1-{1-[(2-Chlorothiazol-5-yl)methyl]-2-[(2-chlorothiazol-5-yl)methylsulfanyl]-4-methyl-6-phenyl-1,6-dihydropyrimidin-5-yl}ethanone

X.-F. Zhu, D.-Q. Shi, F. Luo and Z.-F. Wang

Comment

Biginelli reaction is one of the most powerful synthetic methodologies for the heterocyclic six-membered rings. 3,4-Dihydropyrimidin-2(1*H*)-ones (DHPMs) and their derivatives have attracted considerable interest due to their wide range of therapeutic and pharmacological properties, such as antiviral, antitumor, antibacterial and antiinflammatory properties·(Kappe,1993).

We report here the crystal structure of (I) (Fig. 1), which was synthesized by introducing thiazole rings into a Biginelli Dihydropyrimidine molecular framework. The crystal packing shows that the intermolecular C12—H12A···N3^{i} [symmetry code (i) −*x* + 1,*y* + 1/2,-*z* + 3/2] hydrogen bonds link molecules into rows along the *c* axis,while weak, inversion related C18—H18B···O1^{ii} [symmetry code (ii) *x* − 1,*y*,*z*] hydrogen bonds join parallel rows forming a network, Fig, 2, Table 1.

Experimental

A solution of 1-(4-(4-chlorophenyl)-6-methyl-2-thioxo-1,2,3,4- tetrahydropyrimidin-5-yl)ethanone(2 mmol),2-chloro-5-chloromethyl-thiazole (4 mmol) and potassium carbonate powder (2 mmol) in anhydrous Dimethyl Formamide (10 ml)was stirred vigorously at room temperature until the reaction was complete (monitored by thin-layer chromatography), the solid filtered off and the filtrate concentrated under vacuum·The residue was purified by column chromatography on silica gel using (2:1 *v*/*v*) petroleum ether/ethyl acetate as the eluent, giving a green solid (yield 88%, m.p.412 − 414 K). A yellow crystal grown from dichloromethane and hexane (2:1 *v*/*v*) was selected for X-ray structure analysis.

Refinement

The H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding-model approximation, with U_{iso}(H) = 1.2–1.5U_{eq}(carrier atom). A rotating group model was used for the methyl groups.

Figures

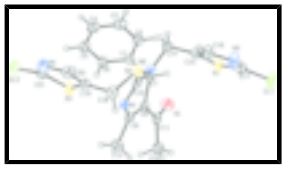

Fig. 1. The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

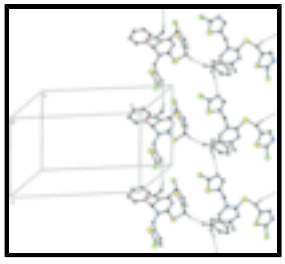

Fig. 2. Crystal packing of (I)·Intermolecular C—H···N and C—H···O interactions (dashed lines). Other H atoms have been omitted for clarity. [Symmetry codes:(i) −*x* + 1,*y* + 1/2,-*z* + 3/2;(ii) *x* − 1,*y*,*z*.]

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Crystal data

$C_{21}H_{18}Cl_2N_4OS_3$	F_{000} = 1048
M_r = 509.47	D_x = 1.492 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 5976 reflections
a = 10.6123 (5) Å	θ = 2.4–27.5º
b = 18.7414 (6) Å	μ = 0.59 mm^{-1}
c = 12.4631 (9) Å	T = 300 (2) K
β = 113.820 (1)º	Block, yellow
V = 2267.6 (2) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4937 independent reflections
Radiation source: fine-focus sealed tube	3980 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.043
T = 300(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Bruker, 2000 or Sheldrick, 2001)	h = −13→13
T_{min} = 0.844, T_{max} = 0.892	k = −23→23
15492 measured reflections	l = −10→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.134	$w = 1/[\sigma^2(F_o^2) + (0.0801P)^2 + 0.0525P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max}$ = 0.001

4937 reflections	$\Delta\rho_{max} = 0.76$ e Å^{-3}
282 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.30256 (19)	0.89461 (10)	0.60611 (17)	0.0352 (4)
C2	0.3048 (2)	0.82610 (11)	0.5661 (2)	0.0465 (5)
H2	0.3766	0.7956	0.6091	0.056*
C3	0.2016 (3)	0.80212 (13)	0.4627 (2)	0.0585 (6)
H3	0.2047	0.7559	0.4368	0.070*
C4	0.0950 (3)	0.84651 (14)	0.3985 (2)	0.0559 (6)
H4	0.0253	0.8303	0.3295	0.067*
C5	0.0913 (2)	0.91513 (13)	0.4365 (2)	0.0513 (5)
H5	0.0194	0.9454	0.3928	0.062*
C6	0.1943 (2)	0.93915 (11)	0.53947 (19)	0.0436 (5)
H6	0.1912	0.9856	0.5645	0.052*
C7	0.41613 (19)	0.92033 (10)	0.71977 (17)	0.0341 (4)
H7	0.4727	0.8789	0.7580	0.041*
C8	0.36497 (19)	0.95276 (10)	0.80526 (16)	0.0330 (4)
C9	0.34482 (19)	1.02505 (10)	0.80124 (17)	0.0346 (4)
C10	0.48273 (19)	1.04236 (10)	0.70042 (16)	0.0351 (4)
C11	0.3459 (2)	0.90123 (11)	0.88574 (18)	0.0396 (5)
C12	0.3194 (3)	0.92329 (14)	0.9906 (2)	0.0549 (6)
H12A	0.2251	0.9378	0.9656	0.082*
H12B	0.3788	0.9624	1.0293	0.082*
H12C	0.3375	0.8838	1.0438	0.082*
C13	0.2709 (3)	1.06632 (12)	0.8610 (2)	0.0512 (6)
H13A	0.2031	1.0363	0.8711	0.077*
H13B	0.2263	1.1069	0.8140	0.077*
H13C	0.3358	1.0822	0.9363	0.077*
C14	0.6133 (2)	0.94307 (12)	0.66158 (19)	0.0425 (5)
H14A	0.6286	0.9759	0.6078	0.051*
H14B	0.5808	0.8984	0.6205	0.051*

C15	0.7465 (2)	0.93043 (11)	0.76409 (19)	0.0429 (5)
C16	0.8646 (2)	0.96685 (15)	0.7921 (2)	0.0635 (7)
H16	0.8723	1.0041	0.7458	0.076*
C17	0.9358 (2)	0.89425 (14)	0.9401 (2)	0.0561 (6)
C18	0.4988 (2)	1.18515 (11)	0.6571 (2)	0.0504 (6)
H18A	0.4788	1.1865	0.7265	0.061*
H18B	0.5626	1.2236	0.6635	0.061*
C19	0.3691 (2)	1.19778 (10)	0.5523 (2)	0.0444 (5)
C20	0.3491 (3)	1.24214 (12)	0.4621 (2)	0.0522 (6)
H20	0.4199	1.2709	0.4608	0.063*
C21	0.1427 (3)	1.19993 (12)	0.3961 (2)	0.0510 (6)
Cl1	1.04156 (7)	0.85525 (5)	1.06951 (7)	0.0834 (3)
Cl2	−0.02682 (7)	1.18481 (4)	0.30615 (7)	0.0712 (2)
N1	0.39481 (17)	1.06949 (8)	0.73819 (15)	0.0377 (4)
N2	0.50686 (16)	0.97250 (8)	0.69595 (14)	0.0356 (4)
N3	0.9741 (2)	0.94605 (14)	0.8934 (2)	0.0749 (7)
N4	0.2201 (2)	1.24354 (10)	0.37161 (18)	0.0582 (5)
O1	0.35742 (19)	0.83736 (9)	0.86936 (16)	0.0620 (5)
S1	0.76960 (6)	0.86607 (3)	0.86811 (6)	0.05590 (19)
S2	0.58141 (5)	1.10075 (3)	0.65412 (5)	0.04610 (17)
S3	0.21580 (6)	1.15434 (3)	0.52678 (6)	0.05366 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0362 (10)	0.0342 (10)	0.0367 (11)	−0.0047 (7)	0.0164 (8)	−0.0023 (8)
C2	0.0535 (13)	0.0363 (11)	0.0498 (13)	0.0007 (9)	0.0211 (11)	−0.0046 (9)
C3	0.0711 (16)	0.0476 (13)	0.0580 (16)	−0.0150 (12)	0.0272 (13)	−0.0215 (12)
C4	0.0561 (14)	0.0641 (15)	0.0430 (14)	−0.0151 (12)	0.0153 (11)	−0.0146 (11)
C5	0.0451 (12)	0.0593 (14)	0.0423 (13)	−0.0012 (10)	0.0100 (10)	0.0003 (11)
C6	0.0421 (11)	0.0376 (11)	0.0459 (13)	0.0001 (8)	0.0122 (10)	−0.0056 (9)
C7	0.0332 (9)	0.0299 (9)	0.0367 (10)	0.0015 (7)	0.0115 (8)	0.0007 (8)
C8	0.0303 (9)	0.0353 (10)	0.0306 (10)	−0.0006 (7)	0.0094 (8)	−0.0009 (8)
C9	0.0315 (9)	0.0368 (10)	0.0317 (10)	−0.0006 (7)	0.0090 (8)	−0.0025 (8)
C10	0.0330 (9)	0.0386 (10)	0.0284 (10)	−0.0053 (7)	0.0069 (8)	0.0019 (8)
C11	0.0310 (10)	0.0444 (12)	0.0389 (11)	0.0000 (8)	0.0093 (8)	0.0055 (9)
C12	0.0532 (13)	0.0699 (16)	0.0433 (13)	0.0006 (11)	0.0213 (11)	0.0117 (11)
C13	0.0591 (14)	0.0440 (12)	0.0570 (15)	0.0039 (10)	0.0302 (12)	−0.0050 (10)
C14	0.0415 (11)	0.0483 (12)	0.0407 (12)	−0.0017 (9)	0.0198 (9)	−0.0052 (9)
C15	0.0399 (11)	0.0490 (12)	0.0439 (12)	0.0029 (9)	0.0211 (10)	−0.0003 (9)
C16	0.0407 (12)	0.0721 (17)	0.0715 (17)	−0.0041 (11)	0.0160 (12)	0.0236 (14)
C17	0.0439 (12)	0.0660 (16)	0.0560 (15)	0.0077 (11)	0.0177 (11)	0.0118 (12)
C18	0.0590 (14)	0.0349 (11)	0.0551 (14)	−0.0140 (9)	0.0206 (11)	−0.0030 (10)
C19	0.0520 (12)	0.0313 (10)	0.0520 (13)	−0.0038 (8)	0.0231 (10)	0.0000 (9)
C20	0.0624 (15)	0.0351 (11)	0.0632 (16)	−0.0009 (10)	0.0296 (13)	0.0074 (10)
C21	0.0603 (14)	0.0382 (11)	0.0506 (14)	0.0060 (10)	0.0184 (11)	0.0074 (10)
Cl1	0.0588 (4)	0.1075 (6)	0.0750 (5)	0.0151 (4)	0.0177 (4)	0.0418 (4)
Cl2	0.0631 (4)	0.0636 (4)	0.0670 (4)	0.0024 (3)	0.0057 (3)	0.0088 (3)

N1	0.0402 (9)	0.0326 (8)	0.0374 (9)	0.0000 (7)	0.0126 (7)	0.0006 (7)
N2	0.0346 (9)	0.0352 (8)	0.0381 (9)	−0.0030 (6)	0.0158 (7)	−0.0025 (7)
N3	0.0450 (12)	0.0864 (17)	0.0816 (17)	−0.0085 (11)	0.0135 (12)	0.0285 (14)
N4	0.0705 (14)	0.0437 (11)	0.0603 (14)	0.0076 (10)	0.0264 (11)	0.0142 (9)
O1	0.0827 (12)	0.0392 (9)	0.0756 (13)	0.0039 (8)	0.0438 (10)	0.0130 (8)
S1	0.0509 (3)	0.0574 (4)	0.0604 (4)	−0.0046 (3)	0.0236 (3)	0.0117 (3)
S2	0.0416 (3)	0.0460 (3)	0.0490 (3)	−0.0067 (2)	0.0164 (2)	0.0080 (2)
S3	0.0523 (3)	0.0485 (3)	0.0548 (4)	−0.0068 (2)	0.0160 (3)	0.0128 (3)

Geometric parameters (Å, °)

C1—C2	1.381 (3)	C12—H12C	0.9600
C1—C6	1.391 (3)	C13—H13A	0.9600
C1—C7	1.521 (3)	C13—H13B	0.9600
C2—C3	1.387 (3)	C13—H13C	0.9600
C2—H2	0.9300	C14—N2	1.468 (3)
C3—C4	1.372 (4)	C14—C15	1.492 (3)
C3—H3	0.9300	C14—H14A	0.9700
C4—C5	1.376 (3)	C14—H14B	0.9700
C4—H4	0.9300	C15—C16	1.344 (3)
C5—C6	1.382 (3)	C15—S1	1.714 (2)
C5—H5	0.9300	C16—N3	1.382 (3)
C6—H6	0.9300	C16—H16	0.9300
C7—N2	1.484 (2)	C17—N3	1.280 (3)
C7—C8	1.506 (3)	C17—S1	1.708 (3)
C7—H7	0.9800	C17—Cl1	1.712 (3)
C8—C9	1.369 (3)	C18—C19	1.485 (3)
C8—C11	1.464 (3)	C18—S2	1.816 (2)
C9—N1	1.389 (2)	C18—H18A	0.9700
C9—C13	1.497 (3)	C18—H18B	0.9700
C10—N1	1.306 (3)	C19—C20	1.344 (3)
C10—N2	1.340 (3)	C19—S3	1.730 (2)
C10—S2	1.7649 (19)	C20—N4	1.378 (3)
C11—O1	1.229 (3)	C20—H20	0.9300
C11—C12	1.501 (3)	C21—N4	1.280 (3)
C12—H12A	0.9600	C21—Cl2	1.716 (3)
C12—H12B	0.9600	C21—S3	1.722 (2)
C2—C1—C6	118.21 (19)	H13A—C13—H13B	109.5
C2—C1—C7	120.55 (18)	C9—C13—H13C	109.5
C6—C1—C7	121.24 (17)	H13A—C13—H13C	109.5
C1—C2—C3	121.0 (2)	H13B—C13—H13C	109.5
C1—C2—H2	119.5	N2—C14—C15	112.58 (17)
C3—C2—H2	119.5	N2—C14—H14A	109.1
C4—C3—C2	120.1 (2)	C15—C14—H14A	109.1
C4—C3—H3	120.0	N2—C14—H14B	109.1
C2—C3—H3	120.0	C15—C14—H14B	109.1
C3—C4—C5	119.8 (2)	H14A—C14—H14B	107.8
C3—C4—H4	120.1	C16—C15—C14	127.1 (2)
C5—C4—H4	120.1	C16—C15—S1	109.09 (18)

C4—C5—C6	120.1 (2)	C14—C15—S1	123.79 (16)
C4—C5—H5	119.9	C15—C16—N3	116.5 (2)
C6—C5—H5	119.9	C15—C16—H16	121.8
C5—C6—C1	120.8 (2)	N3—C16—H16	121.8
C5—C6—H6	119.6	N3—C17—S1	116.4 (2)
C1—C6—H6	119.6	N3—C17—Cl1	123.0 (2)
N2—C7—C8	108.91 (15)	S1—C17—Cl1	120.53 (15)
N2—C7—C1	110.90 (15)	C19—C18—S2	113.85 (16)
C8—C7—C1	114.23 (15)	C19—C18—H18A	108.8
N2—C7—H7	107.5	S2—C18—H18A	108.8
C8—C7—H7	107.5	C19—C18—H18B	108.8
C1—C7—H7	107.5	S2—C18—H18B	108.8
C9—C8—C11	127.94 (18)	H18A—C18—H18B	107.7
C9—C8—C7	117.97 (17)	C20—C19—C18	127.7 (2)
C11—C8—C7	114.07 (16)	C20—C19—S3	108.54 (18)
C8—C9—N1	121.62 (17)	C18—C19—S3	123.73 (16)
C8—C9—C13	126.75 (19)	C19—C20—N4	117.7 (2)
N1—C9—C13	111.63 (17)	C19—C20—H20	121.1
N1—C10—N2	124.88 (17)	N4—C20—H20	121.1
N1—C10—S2	118.76 (15)	N4—C21—Cl2	123.68 (19)
N2—C10—S2	116.34 (15)	N4—C21—S3	117.07 (19)
O1—C11—C8	118.55 (19)	Cl2—C21—S3	119.25 (14)
O1—C11—C12	118.6 (2)	C10—N1—C9	117.53 (16)
C8—C11—C12	122.74 (19)	C10—N2—C14	124.19 (17)
C11—C12—H12A	109.5	C10—N2—C7	119.04 (15)
C11—C12—H12B	109.5	C14—N2—C7	116.66 (16)
H12A—C12—H12B	109.5	C17—N3—C16	109.0 (2)
C11—C12—H12C	109.5	C21—N4—C20	108.3 (2)
H12A—C12—H12C	109.5	C17—S1—C15	88.97 (11)
H12B—C12—H12C	109.5	C10—S2—C18	100.26 (10)
C9—C13—H13A	109.5	C21—S3—C19	88.34 (12)
C9—C13—H13B	109.5		
C6—C1—C2—C3	−0.4 (3)	N2—C10—N1—C9	14.7 (3)
C7—C1—C2—C3	179.9 (2)	S2—C10—N1—C9	−163.91 (14)
C1—C2—C3—C4	−0.1 (4)	C8—C9—N1—C10	−12.2 (3)
C2—C3—C4—C5	0.6 (4)	C13—C9—N1—C10	167.42 (18)
C3—C4—C5—C6	−0.4 (4)	N1—C10—N2—C14	−175.22 (18)
C4—C5—C6—C1	−0.1 (4)	S2—C10—N2—C14	3.4 (2)
C2—C1—C6—C5	0.5 (3)	N1—C10—N2—C7	8.7 (3)
C7—C1—C6—C5	−179.7 (2)	S2—C10—N2—C7	−172.67 (13)
C2—C1—C7—N2	108.2 (2)	C15—C14—N2—C10	92.6 (2)
C6—C1—C7—N2	−71.5 (2)	C15—C14—N2—C7	−91.3 (2)
C2—C1—C7—C8	−128.2 (2)	C8—C7—N2—C10	−30.7 (2)
C6—C1—C7—C8	52.1 (2)	C1—C7—N2—C10	95.8 (2)
N2—C7—C8—C9	32.2 (2)	C8—C7—N2—C14	152.93 (16)
C1—C7—C8—C9	−92.4 (2)	C1—C7—N2—C14	−80.5 (2)
N2—C7—C8—C11	−146.46 (16)	S1—C17—N3—C16	0.4 (3)
C1—C7—C8—C11	88.9 (2)	Cl1—C17—N3—C16	−178.2 (2)
C11—C8—C9—N1	165.72 (18)	C15—C16—N3—C17	−0.2 (4)

C7—C8—C9—N1	−12.7 (3)	Cl2—C21—N4—C20	−179.69 (18)
C11—C8—C9—C13	−13.8 (3)	S3—C21—N4—C20	0.0 (3)
C7—C8—C9—C13	167.71 (19)	C19—C20—N4—C21	0.8 (3)
C9—C8—C11—O1	173.7 (2)	N3—C17—S1—C15	−0.4 (2)
C7—C8—C11—O1	−7.8 (3)	Cl1—C17—S1—C15	178.23 (18)
C9—C8—C11—C12	−9.3 (3)	C16—C15—S1—C17	0.2 (2)
C7—C8—C11—C12	169.16 (18)	C14—C15—S1—C17	−178.51 (19)
N2—C14—C15—C16	−109.7 (3)	N1—C10—S2—C18	−8.43 (18)
N2—C14—C15—S1	68.8 (2)	N2—C10—S2—C18	172.88 (16)
C14—C15—C16—N3	178.6 (2)	C19—C18—S2—C10	−80.61 (18)
S1—C15—C16—N3	−0.1 (3)	N4—C21—S3—C19	−0.6 (2)
S2—C18—C19—C20	−105.1 (2)	Cl2—C21—S3—C19	179.16 (15)
S2—C18—C19—S3	73.8 (2)	C20—C19—S3—C21	0.92 (18)
C18—C19—C20—N4	177.9 (2)	C18—C19—S3—C21	−178.2 (2)
S3—C19—C20—N4	−1.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18A···N1	0.97	2.39	2.799 (3)	105
C14—H14A···S2	0.97	2.51	2.972 (2)	109
C7—H7···O1	0.98	2.32	2.687 (3)	101
C18—H18B···O1^{i}	0.97	2.39	3.314 (3)	159
C12—H12A···N3^{ii}	0.96	2.45	3.390 (3)	167

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*−1, *y*, *z*.

Fig. 1

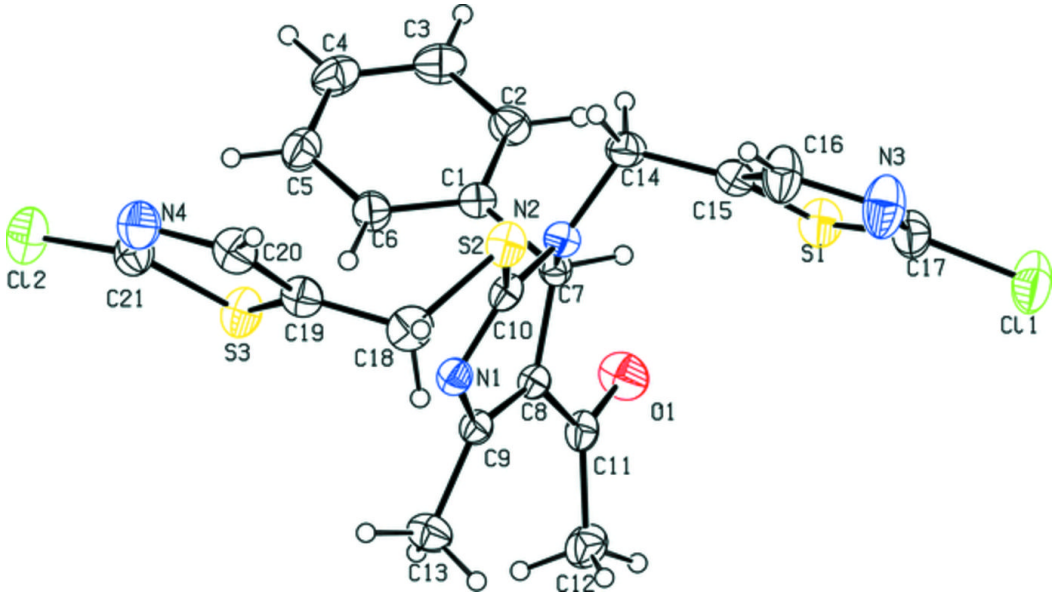
C4
C3
C2
C5
C1
C14
C16
N3
C15
N4
N2
C6
S2
S1
C17
Cl2
C20
C21
C7
Cl1
S3
C19
C10
C18
N1
C8
O1
C9
C11
C13
C12

Fig. 2