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N-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-ylcarbonyl)-*N*′-(2,6-dimethylphenyl)thiourea

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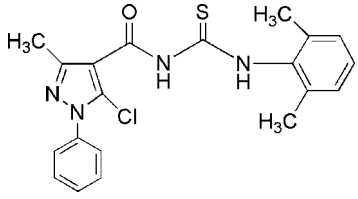
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.090; data-to-parameter ratio = 17.8.

In the title compound, $C_{20}H_{19}ClN_4OS$, the pyrazole ring makes dihedral angles of 89.2 (4) and 46.4 (4)° with the phenyl and substituted benzene rings, respectively; these two six-membered rings are twisted by 52.1 (4)° with respect to each other. There are intramolecular hydrogen bonds of types N—H···O and N—H···Cl.

Related literature

For related literature, see: Du *et al.* (2007); Saeed & Flörke (2007); Wang *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{19}ClN_4OS$
M_r = 398.90
Monoclinic, $P2_1/n$
a = 12.0749 (12) Å
b = 7.6932 (8) Å
c = 21.090 (2) Å
β = 103.071 (4)°
V = 1908.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 113 (2) K
0.32 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.902, T_{max} = 0.950
23102 measured reflections
4554 independent reflections
4164 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.090
S = 1.07
4554 reflections
256 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.87 (2)	1.97 (2)	2.6744 (15)	137 (2)
N2—H2···Cl1	0.82 (2)	2.41 (2)	3.1175 (12)	145 (2)

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2049).

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supplementary materials

Acta Cryst. (2008). E**64**, o157 [**doi:10.1107/S1600536807063544**]

N-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-ylcarbonyl)-*N*'-(2,6-dimethylphenyl)thiourea

H.-T. Du, H.-J. Du, M. Lu and L.-L. Sun

Comment

In the structure of the title compound, (I), the pyrazole ring makes dihedral angles of 89.2 (4) and 46.4 (4)°, with the phenyl rings, C2—C7 and C15—C20, respectively, which are twisted by 52.1 (4)° with respect to each other (Fig. 1). However in a similar structure, *N*-(5-chloro-3-methyl-1-phenyl pyrazole-4-ylcarbonyl)-N' -(4-methphenyl)thiourea (Du *et al.*, 2007), the corresponding phenyl rings from dihedral angles of 74.3 (3) and 2.9 (3)°, respectively, with the central pyrazole system and the dihedral angle between the phenyl rings is 71.6 (3)°. All the bond lengths and angles are in the normal range, corresponding to the related references (Du *et al.*, 2007; Saeed & Flörke, 2007; Wang *et al.*, 2007). The structure is stabilized by N—H···O and N—H···Cl intramolcular hydrogen bonds; details of hydrogen-bonding geometry have been given in the Table.

Experimental

Powdered ammonium thiocyanate (1.14 g, 15 mmol), 5-chloro-3-methyl-1-phenyl-pyrazole-4-carbonyl chloride (2.54 g, 10 mmol), polyethylene glycol-400 (0.5 ml) and acetone (25 ml) were placed in a dried round-bottomed flask containing a magnetic stirrer bar and stirred at room temperature for 1 hr, then 2,6-dimethylbenzenamine (1.15 g, 9.5 mmol) was added, and the mixture was stirred for 5 hr. The mixture was poured into water (20 ml). The resulting solid was filtered, dried and recrystallized from *N*,*N*-dimethylformamide-ethanol (1:1, *v*/*v*) to yield single crystals of (I) by slow evaporation at room temperature.

Refinement

The H-atoms bonded to N-atoms were located from difference map and were allowed to refine freely. All other H atoms were positioned geometrically and included in the refinements using a riding model, with C—H = 0.95 and 0.98 Å and U_{iso}(H) = 1.2 and 1.5 times U_{eq}(C), respectively, for the aromatic and methyl type H-atoms.

Figures

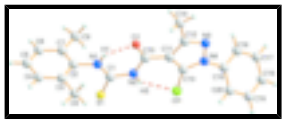


Fig. 1. The molecular structure of (I) with the atomic numbering scheme, showing displacement ellipsoids at 50% probability level. Intramolcular hydrogen bonds have been represented by dashed lines.

N-(5-Chloro-3-methyl-1-phenyl-1*H*-pyrazol-4-ylcarbonyl)-N'- (2,6-dimethylphenyl)thiourea

Crystal data

$C_{20}H_{19}ClN_4OS$	F_{000} = 832
M_r = 398.90	D_x = 1.388 Mg m^{-3}

Monoclinic, $P2_1/n$	Melting point: 459 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
$a = 12.0749\ (12)$ Å	Cell parameters from 5929 reflections
$b = 7.6932\ (8)$ Å	$\theta = 1.8–27.9°$
$c = 21.090\ (2)$ Å	$\mu = 0.33$ mm^{-1}
$\beta = 103.071\ (4)°$	$T = 113\ (2)$ K
$V = 1908.4\ (3)$ Å^3	Prism, colorless
$Z = 4$	0.32 × 0.18 × 0.16 mm

Data collection

Rigaku Saturn diffractometer	4554 independent reflections
Radiation source: rotating anode	4164 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.041$
$T = 113(2)$ K	$\theta_{max} = 27.9°$
ω scans	$\theta_{min} = 1.8°$
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	$h = -15\rightarrow15$
$T_{min} = 0.902$, $T_{max} = 0.950$	$k = -10\rightarrow10$
23102 measured reflections	$l = -26\rightarrow27$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: geom/difmap
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.090$	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.794P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
4554 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
256 parameters	$\Delta\rho_{min} = -0.27$ 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}
Cl1	0.43026 (3)	0.10904 (5)	0.202263 (15)	0.02133 (10)
S1	0.79209 (3)	−0.08648 (5)	0.266243 (16)	0.02236 (10)
O1	0.63163 (9)	0.16452 (16)	0.41897 (5)	0.0287 (3)
N1	0.81514 (9)	0.02276 (15)	0.38858 (5)	0.0172 (2)
N2	0.64393 (10)	0.08216 (15)	0.31685 (6)	0.0169 (2)
N3	0.28650 (10)	0.27287 (16)	0.33684 (5)	0.0194 (2)
N4	0.29269 (9)	0.22644 (15)	0.27493 (5)	0.0165 (2)
C1	0.75248 (11)	0.00996 (17)	0.32786 (6)	0.0160 (3)
C2	0.92637 (11)	−0.05169 (18)	0.40858 (6)	0.0162 (3)
C3	1.02093 (11)	0.05457 (18)	0.41050 (6)	0.0180 (3)
C4	1.12834 (11)	−0.0181 (2)	0.43418 (7)	0.0210 (3)
H4	1.1942	0.0515	0.4367	0.025*
C5	1.14034 (12)	−0.1897 (2)	0.45402 (6)	0.0211 (3)
H5	1.2140	−0.2368	0.4704	0.025*
C6	1.04501 (12)	−0.29323 (19)	0.45006 (6)	0.0198 (3)
H6	1.0541	−0.4117	0.4630	0.024*
C7	0.93592 (11)	−0.22569 (18)	0.42738 (6)	0.0173 (3)
C8	1.00655 (13)	0.23944 (19)	0.38786 (7)	0.0247 (3)
H8A	0.9586	0.2434	0.3437	0.037*
H8B	1.0812	0.2896	0.3879	0.037*
H8C	0.9704	0.3063	0.4172	0.037*
C9	0.83187 (12)	−0.3363 (2)	0.42329 (8)	0.0259 (3)
H9A	0.7848	−0.2863	0.4509	0.039*
H9B	0.8549	−0.4543	0.4382	0.039*
H9C	0.7882	−0.3405	0.3781	0.039*
C10	0.58681 (11)	0.14840 (18)	0.36088 (6)	0.0176 (3)
C11	0.46730 (11)	0.19453 (18)	0.33493 (6)	0.0164 (3)
C12	0.39116 (11)	0.25472 (19)	0.37263 (6)	0.0187 (3)
C13	0.39920 (11)	0.17882 (17)	0.27273 (6)	0.0161 (3)
C14	0.41480 (13)	0.2956 (2)	0.44358 (7)	0.0267 (3)
H14A	0.3477	0.3503	0.4539	0.040*
H14B	0.4796	0.3753	0.4547	0.040*
H14C	0.4326	0.1880	0.4687	0.040*
C15	0.19141 (11)	0.22612 (18)	0.22397 (6)	0.0164 (3)
C16	0.09328 (11)	0.15251 (19)	0.23588 (7)	0.0196 (3)
H16	0.0933	0.1027	0.2771	0.024*
C17	−0.00513 (12)	0.1527 (2)	0.18663 (7)	0.0236 (3)
H17	−0.0735	0.1053	0.1944	0.028*
C18	−0.00365 (12)	0.2219 (2)	0.12628 (7)	0.0247 (3)
H18	−0.0706	0.2192	0.0924	0.030*
C19	0.09488 (12)	0.2950 (2)	0.11495 (7)	0.0233 (3)
H19	0.0954	0.3421	0.0734	0.028*
C20	0.19313 (11)	0.29973 (18)	0.16438 (7)	0.0191 (3)
H20	0.2604	0.3527	0.1573	0.023*
H1	0.7828 (15)	0.073 (2)	0.4168 (9)	0.024 (4)*

H2	0.6098 (16)	0.072 (2)	0.2787 (10)	0.034 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01647 (16)	0.0336 (2)	0.01365 (15)	0.00392 (13)	0.00286 (12)	−0.00437 (12)
S1	0.02202 (18)	0.0291 (2)	0.01609 (17)	0.00740 (14)	0.00459 (13)	−0.00227 (13)
O1	0.0192 (5)	0.0482 (7)	0.0168 (5)	0.0090 (5)	0.0000 (4)	−0.0079 (5)
N1	0.0155 (5)	0.0217 (6)	0.0142 (5)	0.0046 (5)	0.0029 (4)	−0.0010 (4)
N2	0.0141 (5)	0.0235 (6)	0.0124 (5)	0.0036 (4)	0.0012 (4)	0.0006 (4)
N3	0.0177 (6)	0.0266 (6)	0.0141 (5)	0.0026 (5)	0.0043 (4)	−0.0020 (5)
N4	0.0146 (5)	0.0226 (6)	0.0121 (5)	0.0013 (4)	0.0024 (4)	−0.0007 (4)
C1	0.0161 (6)	0.0156 (6)	0.0165 (6)	0.0012 (5)	0.0043 (5)	0.0025 (5)
C2	0.0136 (6)	0.0222 (7)	0.0127 (6)	0.0033 (5)	0.0029 (5)	−0.0007 (5)
C3	0.0191 (6)	0.0215 (7)	0.0143 (6)	0.0007 (5)	0.0056 (5)	−0.0028 (5)
C4	0.0154 (6)	0.0297 (8)	0.0183 (6)	−0.0023 (6)	0.0048 (5)	−0.0065 (6)
C5	0.0148 (6)	0.0325 (8)	0.0152 (6)	0.0063 (6)	0.0014 (5)	−0.0037 (5)
C6	0.0211 (7)	0.0235 (7)	0.0144 (6)	0.0060 (5)	0.0033 (5)	0.0016 (5)
C7	0.0163 (6)	0.0218 (7)	0.0138 (6)	0.0026 (5)	0.0032 (5)	−0.0001 (5)
C8	0.0290 (8)	0.0213 (7)	0.0265 (7)	−0.0014 (6)	0.0116 (6)	−0.0007 (6)
C9	0.0215 (7)	0.0243 (8)	0.0306 (8)	−0.0002 (6)	0.0033 (6)	0.0075 (6)
C10	0.0153 (6)	0.0199 (6)	0.0170 (6)	0.0003 (5)	0.0025 (5)	−0.0007 (5)
C11	0.0151 (6)	0.0191 (7)	0.0145 (6)	0.0011 (5)	0.0024 (5)	−0.0004 (5)
C12	0.0174 (6)	0.0227 (7)	0.0160 (6)	0.0022 (5)	0.0037 (5)	−0.0013 (5)
C13	0.0158 (6)	0.0185 (6)	0.0145 (6)	0.0011 (5)	0.0046 (5)	−0.0001 (5)
C14	0.0216 (7)	0.0412 (9)	0.0168 (7)	0.0047 (6)	0.0035 (5)	−0.0062 (6)
C15	0.0140 (6)	0.0189 (6)	0.0155 (6)	0.0021 (5)	0.0014 (5)	−0.0026 (5)
C16	0.0177 (6)	0.0236 (7)	0.0183 (6)	0.0008 (5)	0.0056 (5)	0.0005 (5)
C17	0.0143 (6)	0.0296 (8)	0.0270 (7)	−0.0014 (6)	0.0047 (6)	−0.0025 (6)
C18	0.0169 (7)	0.0328 (8)	0.0218 (7)	0.0023 (6)	−0.0013 (5)	−0.0021 (6)
C19	0.0209 (7)	0.0295 (8)	0.0178 (6)	0.0033 (6)	0.0012 (5)	0.0032 (6)
C20	0.0155 (6)	0.0224 (7)	0.0191 (6)	0.0004 (5)	0.0031 (5)	0.0014 (5)

Geometric parameters (Å, °)

Cl1—C13	1.6998 (13)	C8—H8A	0.9800
S1—C1	1.6581 (13)	C8—H8B	0.9800
O1—C10	1.2284 (16)	C8—H8C	0.9800
N1—C1	1.3355 (17)	C9—H9A	0.9800
N1—C2	1.4331 (16)	C9—H9B	0.9800
N1—H1	0.87 (2)	C9—H9C	0.9800
N2—C10	1.3738 (17)	C10—C11	1.4665 (18)
N2—C1	1.3939 (17)	C11—C13	1.3869 (18)
N2—H2	0.82 (2)	C11—C12	1.4222 (18)
N3—C12	1.3247 (17)	C12—C14	1.4920 (18)
N3—N4	1.3719 (15)	C14—H14A	0.9800
N4—C13	1.3482 (17)	C14—H14B	0.9800
N4—C15	1.4339 (16)	C14—H14C	0.9800
C2—C7	1.3935 (19)	C15—C20	1.3828 (19)

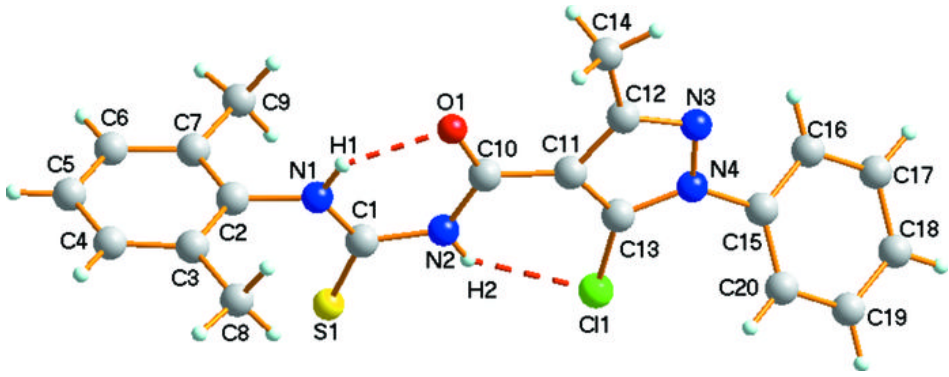
C2—C3	1.3974 (19)	C15—C16	1.3865 (19)
C3—C4	1.3968 (19)	C16—C17	1.3902 (19)
C3—C8	1.498 (2)	C16—H16	0.9500
C4—C5	1.383 (2)	C17—C18	1.383 (2)
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.387 (2)	C18—C19	1.385 (2)
C5—H5	0.9500	C18—H18	0.9500
C6—C7	1.3960 (18)	C19—C20	1.3915 (19)
C6—H6	0.9500	C19—H19	0.9500
C7—C9	1.5038 (19)	C20—H20	0.9500
C1—N1—C2	122.87 (11)	C7—C9—H9C	109.5
C1—N1—H1	116.2 (11)	H9A—C9—H9C	109.5
C2—N1—H1	120.8 (11)	H9B—C9—H9C	109.5
C10—N2—C1	129.21 (11)	O1—C10—N2	122.43 (12)
C10—N2—H2	118.6 (14)	O1—C10—C11	121.48 (12)
C1—N2—H2	111.8 (13)	N2—C10—C11	116.07 (11)
C12—N3—N4	105.34 (11)	C13—C11—C12	103.72 (11)
C13—N4—N3	111.18 (10)	C13—C11—C10	130.91 (12)
C13—N4—C15	129.22 (11)	C12—C11—C10	125.17 (12)
N3—N4—C15	119.54 (10)	N3—C12—C11	111.70 (12)
N1—C1—N2	115.97 (12)	N3—C12—C14	119.38 (12)
N1—C1—S1	125.67 (10)	C11—C12—C14	128.91 (12)
N2—C1—S1	118.35 (10)	N4—C13—C11	108.05 (11)
C7—C2—C3	122.63 (12)	N4—C13—Cl1	121.12 (10)
C7—C2—N1	118.65 (12)	C11—C13—Cl1	130.81 (11)
C3—C2—N1	118.69 (12)	C12—C14—H14A	109.5
C4—C3—C2	117.57 (13)	C12—C14—H14B	109.5
C4—C3—C8	121.68 (13)	H14A—C14—H14B	109.5
C2—C3—C8	120.75 (12)	C12—C14—H14C	109.5
C5—C4—C3	121.03 (13)	H14A—C14—H14C	109.5
C5—C4—H4	119.5	H14B—C14—H14C	109.5
C3—C4—H4	119.5	C20—C15—C16	121.40 (12)
C4—C5—C6	120.10 (13)	C20—C15—N4	119.66 (12)
C4—C5—H5	119.9	C16—C15—N4	118.94 (12)
C6—C5—H5	119.9	C15—C16—C17	119.03 (13)
C5—C6—C7	120.86 (13)	C15—C16—H16	120.5
C5—C6—H6	119.6	C17—C16—H16	120.5
C7—C6—H6	119.6	C18—C17—C16	120.08 (13)
C2—C7—C6	117.78 (13)	C18—C17—H17	120.0
C2—C7—C9	120.86 (12)	C16—C17—H17	120.0
C6—C7—C9	121.36 (13)	C17—C18—C19	120.36 (13)
C3—C8—H8A	109.5	C17—C18—H18	119.8
C3—C8—H8B	109.5	C19—C18—H18	119.8
H8A—C8—H8B	109.5	C18—C19—C20	120.09 (13)
C3—C8—H8C	109.5	C18—C19—H19	120.0
H8A—C8—H8C	109.5	C20—C19—H19	120.0
H8B—C8—H8C	109.5	C15—C20—C19	119.00 (13)
C7—C9—H9A	109.5	C15—C20—H20	120.5
C7—C9—H9B	109.5	C19—C20—H20	120.5

H9A—C9—H9B	109.5		
C12—N3—N4—C13	0.60 (15)	N2—C10—C11—C12	175.91 (13)
C12—N3—N4—C15	177.88 (12)	N4—N3—C12—C11	−0.58 (16)
C2—N1—C1—N2	177.06 (12)	N4—N3—C12—C14	179.86 (13)
C2—N1—C1—S1	−1.7 (2)	C13—C11—C12—N3	0.36 (16)
C10—N2—C1—N1	−7.9 (2)	C10—C11—C12—N3	−174.98 (13)
C10—N2—C1—S1	170.98 (12)	C13—C11—C12—C14	179.87 (15)
C1—N1—C2—C7	−84.89 (16)	C10—C11—C12—C14	4.5 (2)
C1—N1—C2—C3	97.20 (16)	N3—N4—C13—C11	−0.38 (16)
C7—C2—C3—C4	−1.91 (19)	C15—N4—C13—C11	−177.33 (13)
N1—C2—C3—C4	175.92 (11)	N3—N4—C13—Cl1	178.12 (9)
C7—C2—C3—C8	178.10 (12)	C15—N4—C13—Cl1	1.2 (2)
N1—C2—C3—C8	−4.07 (19)	C12—C11—C13—N4	0.02 (15)
C2—C3—C4—C5	0.97 (19)	C10—C11—C13—N4	174.98 (14)
C8—C3—C4—C5	−179.04 (12)	C12—C11—C13—Cl1	−178.29 (11)
C3—C4—C5—C6	0.6 (2)	C10—C11—C13—Cl1	−3.3 (2)
C4—C5—C6—C7	−1.3 (2)	C13—N4—C15—C20	−48.8 (2)
C3—C2—C7—C6	1.24 (19)	N3—N4—C15—C20	134.47 (14)
N1—C2—C7—C6	−176.58 (11)	C13—N4—C15—C16	131.62 (15)
C3—C2—C7—C9	−178.78 (13)	N3—N4—C15—C16	−45.11 (18)
N1—C2—C7—C9	3.40 (19)	C20—C15—C16—C17	0.2 (2)
C5—C6—C7—C2	0.39 (19)	N4—C15—C16—C17	179.73 (12)
C5—C6—C7—C9	−179.59 (13)	C15—C16—C17—C18	1.5 (2)
C1—N2—C10—O1	6.0 (2)	C16—C17—C18—C19	−1.6 (2)
C1—N2—C10—C11	−172.25 (13)	C17—C18—C19—C20	−0.1 (2)
O1—C10—C11—C13	−176.38 (15)	C16—C15—C20—C19	−1.8 (2)
N2—C10—C11—C13	1.9 (2)	N4—C15—C20—C19	178.60 (12)
O1—C10—C11—C12	−2.4 (2)	C18—C19—C20—C15	1.8 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.87 (2)	1.97 (2)	2.6744 (15)	137 (2)
N2—H2···Cl1	0.82 (2)	2.41 (2)	3.1175 (12)	145 (2)

Fig. 1


C14
C12
N3
C16
O1
C9
C6
C7
H1
C10
C11
C17
C5
N1
N4
C1
C18
C4
C2
N2
C13
C15
C3
H2
C20
C8
S1
Cl1
C19