Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(5-Chloro-3-methyl-1-phenylpyrazol-4-ylcarbonyl)-*N*′-(2-methoxyphenyl)thiourea

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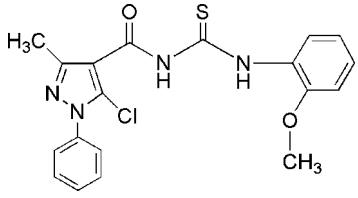
Received 17 November 2007; accepted 25 December 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.098; data-to-parameter ratio = 14.9.

In the title compound, $C_{19}H_{17}ClN_4O_2S$, the dihedral angle between the pyrazole and phenyl rings is 43.3 (3)°. The bridging unit between the pyrazole and methoxyphenyl rings is planar within 0.0169 Å and makes dihedral angles of 2.3 and 26.4°, respectively, with these two rings. This conformation is influenced by intramolecular N—H···O and N—H···Cl hydrogen bonds. The crystal packing is stabilized by C—H···π interactions.

Related literature

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



Experimental

Crystal data

$C_{19}H_{17}ClN_4O_2S$
M_r = 400.88
Monoclinic, $P2_1/c$
a = 20.339 (2) Å
b = 7.4408 (9) Å
c = 12.7919 (15) Å
β = 107.029 (2)°
V = 1851.0 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.941
10087 measured reflections
3793 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.04
3793 reflections
254 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C1–C6 and C13–C18 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3*A*···Cl1	0.890 (9)	2.398 (14)	3.1657 (14)	144.6 (17)
N4—H4*A*···O1	0.895 (9)	1.913 (15)	2.6589 (19)	139.6 (18)
C2—H2···*Cg*1^{i}	0.93	2.88	3.613 (2)	136
C10—H10*B*···*Cg*2^{ii}	0.96	2.98	3.809 (2)	146

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

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

The authors thank Guiyang College (grant No. 2007012) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2053).

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 doi:10.1107/S1600536807068390

supporting information

Acta Cryst. (2008). E**64**, o609 [doi:10.1107/S1600536807068390]

N-(5-Chloro-3-methyl-1-phenylpyrazol-4-ylcarbonyl)-*N*′-(2-methoxyphenyl)-thiourea

Hai-tang Du, Hai-jun Du, Ming Lu and Li-li Sun

S1. Comment

The molecular structure of (I) with the atom-numbering scheme is shown in Fig.1. The pyrazole ring makes dihedral angles of 43.3° and 24.5°, with C1—C6 and C13—C18 rings, respectively; these two six-membered rings are twisted by 19.6° with respect to each other. However, in the similar structure, *N*-(5-chloro-3-methyl-1-phenyl pyrazole-4-yl-carbonyl)-*N*′-(4-methphenyl)thiourea (Du *et al.*, 2007), the two phenyl rings deviate from the central pyrazole system with dihedral angles of 74.3° and 2.9°, respectively, the dihedral angle between them being 71.6°. 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). There also exist two intramolecular N—H···O and N—H···Cl hydrogen bonds and two C—H···pi interaction (Table 1.). Investigation on the packing pattern demonstrates that those discrete molecules are interconnected by slightly weak contacts C2—H2···*Cg*1 and C10—H10B···*Cg*2 [*Cg*1=C1—C6 and *Cg*2=C13—C18] into a two-dimensional network, as shown in Fig. 2.

S2. Experimental

Powdered ammonium thiocyanate (15 mmol), 5-chloro-3-methyl-1-phenyl-pyrazole-4-carbonyl chloride (10 mmol), PEG-400 (0.15 mmol) and acetone (25 mL) were placed in a dried round-bottomed flask containing a magnetic stirrer bar and stirred at room temperature for 1 h. Then 2-methoxybenzenamine (9.5 mmol) was added, and the mixture was stirred for 5 h. The mixture was poured into water (20 mL). The resulting solid was filtered, dried and recrystallized from DMF-EtOH to give *N*-(5-chloro-3-methyl-1-phenyl pyrazole-4-ylcarbonyl)-*N*′-(2-methoxyphenyl)thiourea. Single crystals of the title compound were obtained by slow evaporation of a solution in DMF-EtOH(1:1,*v*/*v*).

S3. Refinement

H atoms bonded to N atoms were located in a difference map and refined with distance restraint of N—H = 0.89 Å with U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.2 (1.5 for methyl groups) times U_{eq}(C).

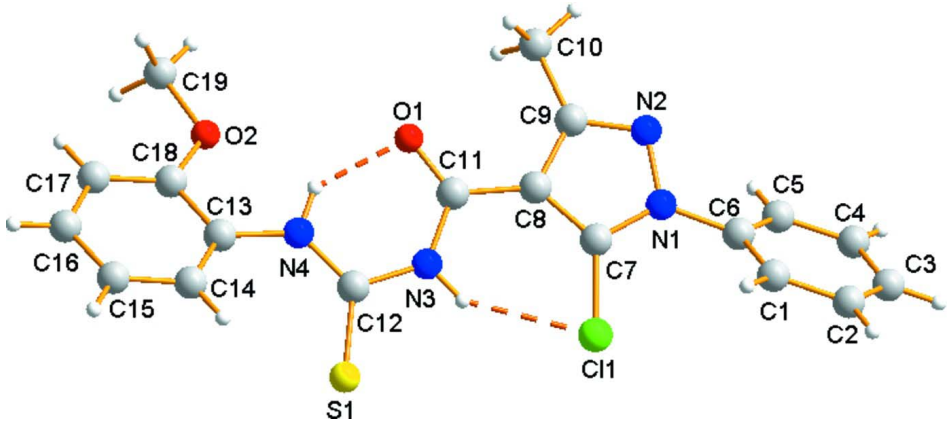

Figure 1

The molecular structure of (I) with the atom numbering scheme, showing N—H···O and N—H···Cl intramolecular hydrogen bonds.

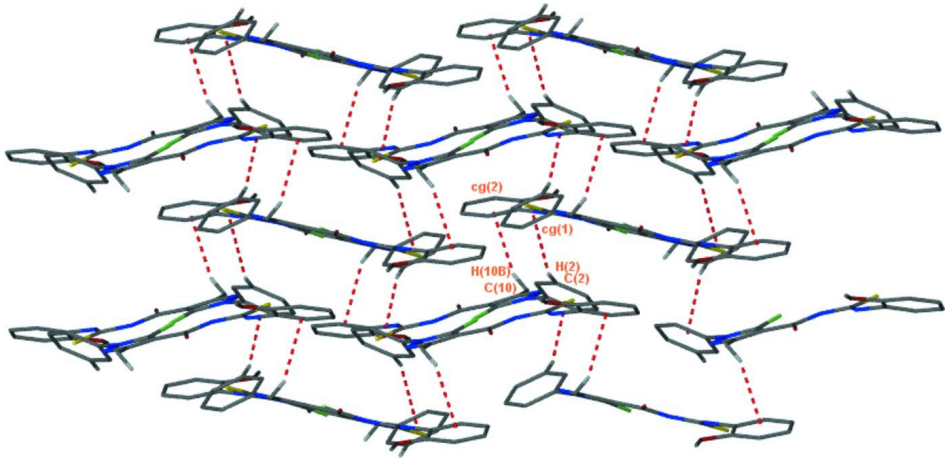

Figure 2

The two-dimensional supramolecular framework showing the C—H···pi contacts [*Cg*1=C1—C6, *Cg*2=C13—C18].

N-(5-Chloro-3-methyl-1-phenylpyrazol-4-ylcarbonyl)- *N*′-(2-methoxyphenyl)thiourea

Crystal data

$C_{19}H_{17}ClN_4O_2S$
$M_r = 400.88$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 20.339\ (2)$ Å
$b = 7.4408\ (9)$ Å
$c = 12.7919\ (15)$ Å
$\beta = 107.029\ (2)°$
$V = 1851.0\ (4)$ Å^3
$Z = 4$

$F(000) = 832$
$D_x = 1.439$ Mg m^{-3}
Melting point: 437 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5493 reflections
$\theta = 2.7–26.4°$
$\mu = 0.34$ mm^{-1}
$T = 294$ K
Prism, colorless
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.941
10087 measured reflections
3793 independent reflections
3065 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.4°, θ_{min} = 2.1°
h = −19→25
k = −9→7
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.097
S = 1.04
3793 reflections
254 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.4744P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.32848 (2)	0.38045 (8)	0.78067 (4)	0.05368 (16)
Cl1	0.39634 (2)	0.49010 (7)	0.47794 (3)	0.04935 (14)
O1	0.16432 (6)	0.5391 (2)	0.46861 (10)	0.0554 (4)
O2	0.06377 (6)	0.3605 (2)	0.62638 (10)	0.0530 (3)
N1	0.32052 (6)	0.59589 (19)	0.27986 (10)	0.0375 (3)
N2	0.25436 (7)	0.6246 (2)	0.21555 (11)	0.0419 (3)
N3	0.27109 (7)	0.4682 (2)	0.57720 (11)	0.0438 (4)
N4	0.19402 (7)	0.4401 (2)	0.67699 (11)	0.0418 (3)
C1	0.43578 (9)	0.6916 (3)	0.27971 (15)	0.0472 (4)
H1	0.4428	0.7452	0.3478	0.057*
C2	0.48659 (9)	0.6974 (3)	0.22681 (16)	0.0523 (5)
H2	0.5284	0.7528	0.2607	0.063*
C3	0.47554 (9)	0.6224 (3)	0.12530 (16)	0.0520 (5)
H3	0.5097	0.6276	0.0905	0.062*
C4	0.41394 (10)	0.5393 (3)	0.07479 (15)	0.0542 (5)

H4	0.4064	0.4903	0.0054	0.065*
C5	0.36327 (9)	0.5282 (3)	0.12681 (14)	0.0472 (4)
H5	0.3220	0.4700	0.0934	0.057*
C6	0.37472 (8)	0.6047 (2)	0.22901 (13)	0.0371 (4)
C7	0.32183 (8)	0.5520 (2)	0.38253 (13)	0.0357 (3)
C8	0.25474 (8)	0.5552 (2)	0.38879 (13)	0.0363 (4)
C9	0.21508 (8)	0.6007 (2)	0.28072 (13)	0.0384 (4)
C10	0.13868 (8)	0.6187 (3)	0.23440 (15)	0.0495 (5)
H10A	0.1276	0.6539	0.1590	0.074*
H10B	0.1223	0.7082	0.2747	0.074*
H10C	0.1172	0.5055	0.2398	0.074*
C11	0.22584 (8)	0.5214 (2)	0.47961 (13)	0.0387 (4)
C12	0.25973 (8)	0.4323 (2)	0.67773 (13)	0.0378 (4)
C13	0.16530 (8)	0.4213 (2)	0.76497 (13)	0.0389 (4)
C14	0.20047 (9)	0.4519 (3)	0.87383 (14)	0.0521 (5)
H14	0.2469	0.4816	0.8937	0.063*
C15	0.16671 (11)	0.4384 (3)	0.95325 (15)	0.0604 (5)
H15	0.1905	0.4596	1.0262	0.072*
C16	0.09837 (11)	0.3938 (3)	0.92464 (16)	0.0601 (5)
H16	0.0763	0.3822	0.9785	0.072*
C17	0.06196 (9)	0.3661 (3)	0.81632 (16)	0.0516 (5)
H17	0.0154	0.3379	0.7973	0.062*
C18	0.09501 (8)	0.3806 (2)	0.73614 (14)	0.0404 (4)
C19	−0.00924 (9)	0.3381 (4)	0.59165 (18)	0.0673 (6)
H19A	−0.0211	0.2307	0.6236	0.101*
H19B	−0.0251	0.3286	0.5134	0.101*
H19C	−0.0305	0.4398	0.6146	0.101*
H3A	0.3155 (5)	0.467 (3)	0.5812 (17)	0.062 (6)*
H4A	0.1642 (8)	0.468 (3)	0.6123 (10)	0.057 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0354 (2)	0.0762 (4)	0.0463 (3)	0.0095 (2)	0.00703 (19)	0.0106 (2)
Cl1	0.0290 (2)	0.0731 (3)	0.0433 (2)	0.00205 (19)	0.00649 (17)	0.0023 (2)
O1	0.0294 (6)	0.0926 (11)	0.0459 (7)	0.0051 (6)	0.0140 (5)	0.0108 (7)
O2	0.0300 (6)	0.0846 (10)	0.0443 (7)	−0.0058 (6)	0.0108 (5)	−0.0054 (6)
N1	0.0276 (6)	0.0478 (8)	0.0377 (7)	−0.0009 (6)	0.0107 (5)	−0.0008 (6)
N2	0.0298 (7)	0.0543 (9)	0.0407 (7)	0.0017 (6)	0.0090 (6)	0.0021 (6)
N3	0.0279 (7)	0.0655 (10)	0.0395 (7)	0.0010 (7)	0.0124 (6)	0.0038 (7)
N4	0.0289 (7)	0.0627 (10)	0.0338 (7)	−0.0018 (6)	0.0092 (6)	0.0016 (7)
C1	0.0395 (9)	0.0516 (11)	0.0540 (10)	−0.0062 (8)	0.0190 (8)	−0.0106 (9)
C2	0.0363 (9)	0.0572 (12)	0.0672 (12)	−0.0069 (8)	0.0213 (8)	−0.0031 (10)
C3	0.0426 (10)	0.0635 (12)	0.0583 (11)	0.0045 (9)	0.0280 (9)	0.0085 (9)
C4	0.0472 (10)	0.0780 (14)	0.0410 (9)	0.0036 (10)	0.0186 (8)	0.0000 (9)
C5	0.0358 (9)	0.0651 (12)	0.0402 (9)	−0.0021 (8)	0.0104 (7)	−0.0014 (8)
C6	0.0302 (8)	0.0418 (9)	0.0420 (8)	0.0022 (7)	0.0146 (7)	0.0029 (7)
C7	0.0283 (7)	0.0413 (9)	0.0364 (8)	−0.0011 (7)	0.0077 (6)	−0.0023 (7)

C8	0.0277 (7)	0.0434 (9)	0.0384 (8)	−0.0007 (7)	0.0108 (6)	−0.0019 (7)
C9	0.0305 (8)	0.0438 (9)	0.0410 (8)	0.0001 (7)	0.0109 (7)	−0.0012 (7)
C10	0.0304 (9)	0.0670 (13)	0.0493 (10)	0.0014 (8)	0.0092 (7)	0.0046 (9)
C11	0.0306 (8)	0.0474 (10)	0.0389 (8)	−0.0011 (7)	0.0112 (7)	−0.0011 (7)
C12	0.0328 (8)	0.0422 (9)	0.0386 (8)	−0.0018 (7)	0.0106 (7)	−0.0003 (7)
C13	0.0348 (8)	0.0462 (10)	0.0382 (8)	0.0029 (7)	0.0145 (7)	0.0031 (7)
C14	0.0394 (9)	0.0748 (14)	0.0413 (9)	0.0019 (9)	0.0104 (8)	−0.0019 (9)
C15	0.0569 (12)	0.0878 (16)	0.0365 (9)	0.0121 (11)	0.0137 (9)	0.0016 (10)
C16	0.0612 (12)	0.0812 (15)	0.0474 (10)	0.0082 (11)	0.0306 (10)	0.0100 (10)
C17	0.0407 (9)	0.0642 (13)	0.0559 (11)	0.0001 (9)	0.0236 (8)	0.0053 (9)
C18	0.0362 (8)	0.0450 (10)	0.0416 (9)	0.0015 (7)	0.0140 (7)	0.0014 (7)
C19	0.0344 (10)	0.0985 (18)	0.0654 (13)	−0.0134 (10)	0.0090 (9)	−0.0023 (12)

Geometric parameters (Å, º)

S1—C12	1.6612 (17)	C4—H4	0.9300
Cl1—C7	1.7072 (16)	C5—C6	1.382 (2)
O1—C11	1.2246 (19)	C5—H5	0.9300
O2—C18	1.369 (2)	C7—C8	1.390 (2)
O2—C19	1.430 (2)	C8—C9	1.422 (2)
N1—C7	1.346 (2)	C8—C11	1.469 (2)
N1—N2	1.3729 (18)	C9—C10	1.498 (2)
N1—C6	1.4361 (19)	C10—H10A	0.9600
N2—C9	1.325 (2)	C10—H10B	0.9600
N3—C11	1.374 (2)	C10—H10C	0.9600
N3—C12	1.397 (2)	C13—C14	1.385 (2)
N3—H3A	0.890 (9)	C13—C18	1.401 (2)
N4—C12	1.335 (2)	C14—C15	1.386 (3)
N4—C13	1.419 (2)	C14—H14	0.9300
N4—H4A	0.895 (9)	C15—C16	1.370 (3)
C1—C6	1.382 (2)	C15—H15	0.9300
C1—C2	1.392 (2)	C16—C17	1.382 (3)
C1—H1	0.9300	C16—H16	0.9300
C2—C3	1.370 (3)	C17—C18	1.385 (2)
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.377 (3)	C19—H19A	0.9600
C3—H3	0.9300	C19—H19B	0.9600
C4—C5	1.383 (2)	C19—H19C	0.9600
C18—O2—C19	117.33 (14)	C8—C9—C10	129.27 (14)
C7—N1—N2	110.99 (12)	C9—C10—H10A	109.5
C7—N1—C6	130.88 (13)	C9—C10—H10B	109.5
N2—N1—C6	117.99 (13)	H10A—C10—H10B	109.5
C9—N2—N1	105.54 (13)	C9—C10—H10C	109.5
C11—N3—C12	130.06 (14)	H10A—C10—H10C	109.5
C11—N3—H3A	117.0 (13)	H10B—C10—H10C	109.5
C12—N3—H3A	112.6 (13)	O1—C11—N3	121.70 (15)
C12—N4—C13	129.34 (14)	O1—C11—C8	121.50 (15)

C12—N4—H4A	114.9 (13)	N3—C11—C8	116.80 (14)
C13—N4—H4A	115.6 (13)	N4—C12—N3	114.84 (14)
C6—C1—C2	118.66 (17)	N4—C12—S1	128.64 (13)
C6—C1—H1	120.7	N3—C12—S1	116.50 (12)
C2—C1—H1	120.7	C14—C13—C18	119.13 (15)
C3—C2—C1	120.60 (17)	C14—C13—N4	124.74 (15)
C3—C2—H2	119.7	C18—C13—N4	115.98 (14)
C1—C2—H2	119.7	C13—C14—C15	120.26 (17)
C2—C3—C4	120.13 (17)	C13—C14—H14	119.9
C2—C3—H3	119.9	C15—C14—H14	119.9
C4—C3—H3	119.9	C16—C15—C14	120.21 (18)
C3—C4—C5	120.31 (18)	C16—C15—H15	119.9
C3—C4—H4	119.8	C14—C15—H15	119.9
C5—C4—H4	119.8	C15—C16—C17	120.51 (17)
C6—C5—C4	119.20 (17)	C15—C16—H16	119.7
C6—C5—H5	120.4	C17—C16—H16	119.7
C4—C5—H5	120.4	C16—C17—C18	119.80 (17)
C5—C6—C1	121.07 (15)	C16—C17—H17	120.1
C5—C6—N1	118.09 (14)	C18—C17—H17	120.1
C1—C6—N1	120.82 (15)	O2—C18—C17	124.80 (15)
N1—C7—C8	108.23 (13)	O2—C18—C13	115.14 (14)
N1—C7—Cl1	121.51 (11)	C17—C18—C13	120.06 (16)
C8—C7—Cl1	130.10 (13)	O2—C19—H19A	109.5
C7—C8—C9	103.59 (13)	O2—C19—H19B	109.5
C7—C8—C11	132.02 (14)	H19A—C19—H19B	109.5
C9—C8—C11	124.40 (14)	O2—C19—H19C	109.5
N2—C9—C8	111.64 (13)	H19A—C19—H19C	109.5
N2—C9—C10	119.07 (15)	H19B—C19—H19C	109.5

C7—N1—N2—C9	1.05 (18)	C11—C8—C9—C10	−2.0 (3)
C6—N1—N2—C9	177.15 (14)	C12—N3—C11—O1	−2.6 (3)
C6—C1—C2—C3	1.6 (3)	C12—N3—C11—C8	177.70 (17)
C1—C2—C3—C4	−0.4 (3)	C7—C8—C11—O1	176.78 (18)
C2—C3—C4—C5	−1.1 (3)	C9—C8—C11—O1	−3.6 (3)
C3—C4—C5—C6	1.3 (3)	C7—C8—C11—N3	−3.5 (3)
C4—C5—C6—C1	0.0 (3)	C9—C8—C11—N3	176.15 (16)
C4—C5—C6—N1	178.21 (16)	C13—N4—C12—N3	−176.04 (17)
C2—C1—C6—C5	−1.4 (3)	C13—N4—C12—S1	5.8 (3)
C2—C1—C6—N1	−179.60 (16)	C11—N3—C12—N4	4.6 (3)
C7—N1—C6—C5	134.17 (19)	C11—N3—C12—S1	−176.95 (15)
N2—N1—C6—C5	−41.0 (2)	C12—N4—C13—C14	23.6 (3)
C7—N1—C6—C1	−47.6 (3)	C12—N4—C13—C18	−160.93 (18)
N2—N1—C6—C1	137.20 (17)	C18—C13—C14—C15	1.4 (3)
N2—N1—C7—C8	−1.46 (19)	N4—C13—C14—C15	176.77 (19)
C6—N1—C7—C8	−176.90 (16)	C13—C14—C15—C16	0.3 (3)
N2—N1—C7—Cl1	174.41 (12)	C14—C15—C16—C17	−1.5 (3)
C6—N1—C7—Cl1	−1.0 (3)	C15—C16—C17—C18	1.0 (3)
N1—C7—C8—C9	1.22 (18)	C19—O2—C18—C17	5.6 (3)

Cl1—C7—C8—C9	−174.18 (14)	C19—O2—C18—C13	−173.48 (18)
N1—C7—C8—C11	−179.09 (17)	C16—C17—C18—O2	−178.28 (19)
Cl1—C7—C8—C11	5.5 (3)	C16—C17—C18—C13	0.7 (3)
N1—N2—C9—C8	−0.24 (19)	C14—C13—C18—O2	177.16 (17)
N1—N2—C9—C10	−178.72 (16)	N4—C13—C18—O2	1.4 (2)
C7—C8—C9—N2	−0.61 (19)	C14—C13—C18—C17	−1.9 (3)
C11—C8—C9—N2	179.67 (16)	N4—C13—C18—C17	−177.68 (17)
C7—C8—C9—C10	177.68 (18)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···Cl1	0.89 (1)	2.40 (1)	3.1657 (14)	145 (2)
N4—H4*A*···O1	0.90 (1)	1.91 (2)	2.6589 (19)	140 (2)
C2—H2···*Cg*1^{i}	0.93	2.88	3.613 (2)	136
C10—H10*B*···*Cg*2^{ii}	0.96	2.98	3.809 (2)	146

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