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1-(2-Chloro-5-nitrophenyl)-3-(2,2-dimethylpropionyl)thiourea

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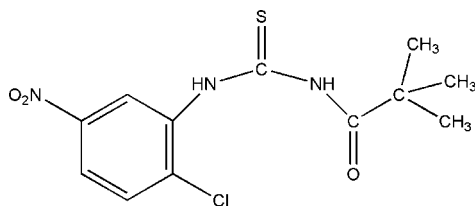
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 Key indicators: single-crystal X-ray study; $T = 89$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.092; data-to-parameter ratio = 11.0.

With the exception of the C atoms of two of the methyl groups of the *tert*-butyl substituent, all of the non-H atoms of the title compound, $\text{C}_{12}\text{H}_{14}\text{ClN}_3\text{O}_3\text{S}$, lie on a mirror plane. The 2-chloro-5-nitrophenyl and 2,2-dimethylpropionyl substituents are, respectively, *cis* and *trans* relative to the thiocarbonyl S atom across the two C–N bonds. Intramolecular N–H···O and C–H···S hydrogen bonds form $S(6)$ ring motifs, also in the mirror plane. Despite the presence of two N–H substituents, no intermolecular hydrogen bonds are observed in the crystal structure. Weak π – π contacts [centroid–centroid distances of 4.2903 (17) Å] involving adjacent aromatic rings link the molecules in a head-to-tail fashion above and below the molecular plane.

Related literature

For the use of thiourea derivatives in organic synthesis, see: Eynde & Watte (2003); Fu *et al.* (1999); Rashdan *et al.* (2006); Maryanoff *et al.* (1986); Wang *et al.* (2005); Saeed *et al.* (2008); and in analysis, see: Koch (2001). For their bioactivity and pharmaceutical applications, see: Upadhyaya & Srivastava (1982); Krishnamurthy *et al.* (1999); Blum & Hayes (1979); DeBeer *et al.* (1936). For related structures, see: Saeed & Flörke (2007*a,b*); Yusof *et al.* (2006, 2008). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{12}\text{H}_{14}\text{ClN}_3\text{O}_3\text{S}$
 $M_r = 315.77$
 Orthorhombic, *Pnma*
 $a = 9.529$ (2) Å
 $b = 6.546$ (2) Å
 $c = 22.166$ (6) Å
 $V = 1382.7$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.44$ mm⁻¹
 $T = 89$ K
 $0.36 \times 0.09 \times 0.06$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2006)
 $T_{\min} = 0.833$, $T_{\max} = 0.974$
 12525 measured reflections
 1434 independent reflections
 1166 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.092$
 $S = 1.09$
 1434 reflections
 130 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.27$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9–H9···S1	0.95	2.51	3.197 (3)	130
N2–H2N···O1	0.97 (3)	1.82 (3)	2.653 (3)	141 (3)

Data collection: APEX2 (Bruker, 2006); cell refinement: APEX2 and SAINT (Bruker, 2006); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008) and TITAN2000 (Hunter & Simpson, 1999); molecular graphics: SHELXTL (Sheldrick, 2008) and Mercury (Macrae *et al.*, 2006); software used to prepare material for publication: SHELXL97, enCIFer (Allen *et al.*, 2004), PLATON (Spek, 2009) and publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2851).

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supporting information

Acta Cryst. (2009). E65, o1735–o1736 [doi:10.1107/S1600536809024672]

1-(2-Chloro-5-nitrophenyl)-3-(2,2-dimethylpropionyl)thiourea

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S1. Comment

Substituted thioureas are versatile building blocks for the synthesis of a variety of heterocyclic compounds with a broad range of useful applications and exhibiting a wide range of bioactivity. Solid-phase Biginelli pyrimidine synthesis (Eynde & Watte, 2003) and synthesis of imidazoline derivatives (Fu *et al.*, 1999) have been carried out using resin-bound thioureas. Pyridyl thioureas are switchable anion receptors (Rashdan *et al.*, 2006); thioureas are also efficient guanylation agents (Maryanoff *et al.*, 1986) while *N,N*-dialkyl-*N*-aroyl thioureas are efficient ligands for the separation of platinum group metals (Koch, 2001). Acyl thioureas are well known for their superior pesticidal, fungicidal, antiviral and plant-growth regulatory activities (Upadhyaya & Srivastava, 1982). 1,3-Dialkyl or diaryl thioureas show powerful antifungal activity against plant pathogens *Pyricularia oryzae* and *Drechslera oryzae* (Krishnamurthy *et al.*, 1999). Substituted thioureas are potent enhancers of 30S dynein ATPase activity and inhibitors of 14S dynein ATPase activity (Blum & Hayes, 1979). Aryl and alkyl-aryl thioureas display strong hypnotic potency in mice (DeBeer *et al.*, 1936). 1-Aroyl-3-arylthioureas are an exceptionally important group of thioureas which have attracted recent interest. They have been used in the synthesis of imidazole-2-thiones (Wang *et al.*, 2005) and 2-(aroylimino)-3-aryl-4-phenyl-1,3-thiazolines (Saeed *et al.*, 2008). We report here the structure of the title thiourea derivative (I), Fig. 1.

With the exception of the C12 atoms of two methyl groups of the *t*-butyl substituent all of the non-hydrogen atoms of the title compound, C₁₃H₁₅N₂O₃SCl lie on a mirror plane. Intramolecular N2—H2N \cdots O1 and C9—H9 \cdots S1 hydrogen bonds each form a 6-membered ring, also in the mirror plane. Bond distances within the molecule are normal (Allen *et al.* 1987) and similar to those observed in comparable structures (Saeed & Flörke 2007a,b; Yusof *et al.* 2006, 2008). Despite the presence of both amide and thioamide groups in the molecule, no intermolecular hydrogen bonds are observed in the crystal structure. Weak π – π contacts between neighbouring C4 \cdots C9 rings, Fig 2, with centroid \cdots centroid distances 4.2903 (17)Å and perpendicular distances between the molecular planes of 3.273Å link adjacent molecules above and below the molecular plane along *b*. These stacks of molecules form sheets parallel to the *c* axis, Fig. 3.

S2. Experimental

A solution of pivaloyl chloride (10 mmol) in anhydrous acetone (50 ml) was added dropwise to a suspension of potassium thiocyanate (10 mmol) in acetone (30 ml) and the reaction mixture was refluxed for 30 min. After cooling to room temperature, a solution of 2-chloro-5-nitroaniline (1.28 g, 10 mmol) in acetone (10 ml) was added and the resulting mixture refluxed for 2 h. The reaction mixture was poured into cold water and the thiourea was precipitated as a white solid. Recrystallization from ethanol gave colorless crystals of (I) (8.6 mmol, 86%). IR (KBr) cm⁻¹: 3351 (free NH), 3200 (assoc. NH), 1667 (CO), 1610 (arom.), 1529 (thioureido I) 1325 II, 1160 III, 744, 762.

S3. Refinement

The H atoms bound to N1 and N2 and C11 were located in a difference Fourier map and their coordinates refined with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{N/C})$. All other H atoms were refined using a riding model with $d(\text{C}-\text{H}) = 0.95 \text{ \AA}$, for aromatic H atoms with $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$. For the remaining methyl groups $d(\text{C}-\text{H}) = 0.98 \text{ \AA}$, $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$.

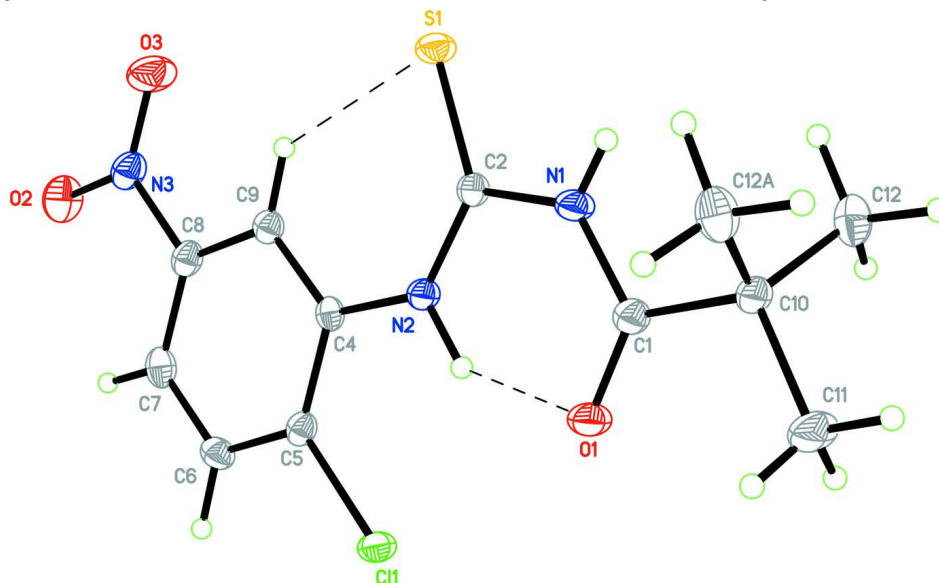


Figure 1

The structure of (I) with displacement ellipsoids for the non-hydrogen atoms drawn at the 50% probability level. Intramolecular hydrogen bonds are drawn as dashed lines. The atom labeled C12A is related to the C12 atom by the symmetry operation $x, -y + 1/2, z$.

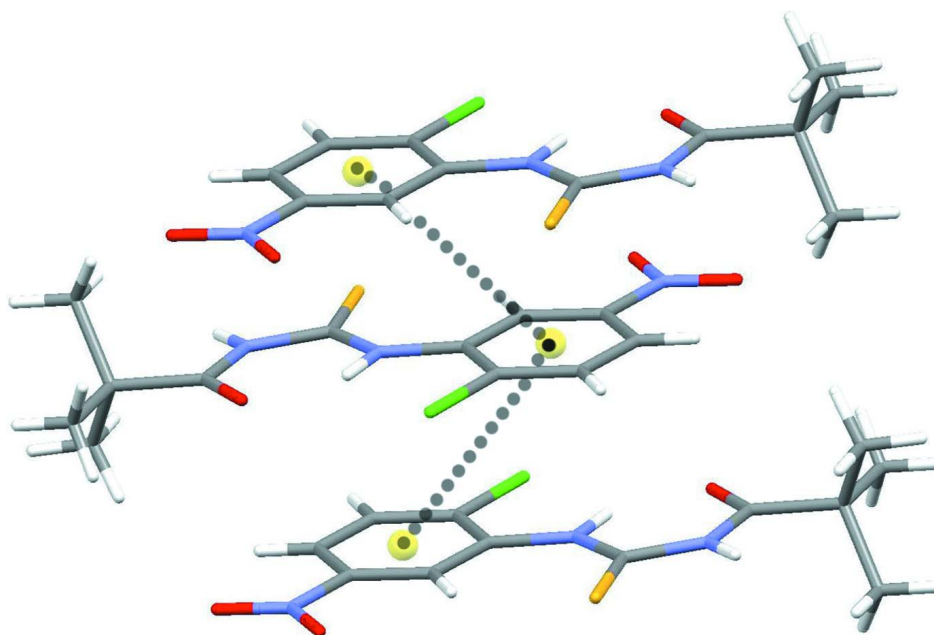
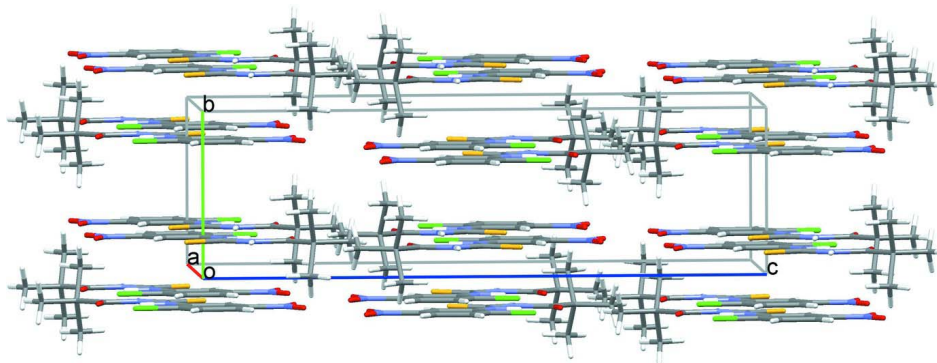


Figure 2

π - π interactions for (1).

**Figure 3**

Crystal packing for (I) viewed down the *a* axis.

1-(2-Chloro-5-nitrophenyl)-3-(2,2-dimethylpropanoyl)thiourea

Crystal data

$C_{12}H_{14}ClN_3O_3S$
 $M_r = 315.77$
 Orthorhombic, *Pnma*
 Hall symbol: -P 2ac 2n
 $a = 9.529 (2) \text{ \AA}$
 $b = 6.546 (2) \text{ \AA}$
 $c = 22.166 (6) \text{ \AA}$
 $V = 1382.7 (7) \text{ \AA}^3$
 $Z = 4$

$F(000) = 656$
 $D_x = 1.517 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 2410 reflections
 $\theta = 2.3\text{--}24.6^\circ$
 $\mu = 0.44 \text{ mm}^{-1}$
 $T = 89 \text{ K}$
 Needle, colourless
 $0.36 \times 0.09 \times 0.06 \text{ mm}$

Data collection

Bruker APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2006)
 $T_{\min} = 0.833$, $T_{\max} = 0.974$

12525 measured reflections
 1434 independent reflections
 1166 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\max} = 25.7^\circ$, $\theta_{\min} = 1.8^\circ$
 $h = -11 \rightarrow 11$
 $k = -6 \rightarrow 8$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.092$
 $S = 1.09$
 1434 reflections
 130 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
 $w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.3426P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1946 (3)	0.2500	0.36075 (12)	0.0163 (6)
O1	0.3187 (2)	0.2500	0.34713 (8)	0.0217 (5)
N1	0.1523 (3)	0.2500	0.42088 (10)	0.0184 (5)
H1N	0.070 (4)	0.2500	0.4268 (16)	0.037 (11)*
C2	0.2314 (3)	0.2500	0.47417 (11)	0.0143 (6)
S1	0.14289 (7)	0.2500	0.53901 (3)	0.0192 (2)
N2	0.3713 (2)	0.2500	0.46466 (10)	0.0143 (5)
H2N	0.397 (3)	0.2500	0.4222 (15)	0.030 (9)*
C4	0.4846 (3)	0.2500	0.50580 (12)	0.0130 (6)
C5	0.6210 (3)	0.2500	0.48174 (11)	0.0147 (6)
C11	0.64439 (7)	0.2500	0.40389 (3)	0.0181 (2)
C6	0.7399 (3)	0.2500	0.51801 (12)	0.0168 (6)
H6	0.8305	0.2500	0.5002	0.020*
C7	0.7261 (3)	0.2500	0.58025 (12)	0.0183 (6)
H7	0.8060	0.2500	0.6059	0.022*
C8	0.5911 (3)	0.2500	0.60368 (11)	0.0167 (6)
N3	0.5743 (3)	0.2500	0.67027 (10)	0.0204 (5)
O2	0.6808 (2)	0.2500	0.70124 (9)	0.0286 (5)
O3	0.4544 (2)	0.2500	0.69074 (9)	0.0317 (6)
C9	0.4711 (3)	0.2500	0.56877 (11)	0.0147 (6)
H9	0.3810	0.2500	0.5871	0.018*
C10	0.0727 (3)	0.2500	0.31561 (11)	0.0170 (6)
C11	0.1330 (3)	0.2500	0.25185 (13)	0.0308 (8)
H11A	0.059 (4)	0.2500	0.2261 (16)	0.037*
H11B	0.188 (2)	0.132 (3)	0.2442 (10)	0.037*
C12	-0.0158 (2)	0.0571 (3)	0.32488 (9)	0.0229 (5)
H12A	-0.0897	0.0515	0.2942	0.034*
H12B	-0.0585	0.0602	0.3651	0.034*
H12C	0.0442	-0.0638	0.3213	0.034*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0149 (14)	0.0200 (15)	0.0142 (14)	0.000	-0.0001 (11)	0.000
O1	0.0135 (10)	0.0360 (12)	0.0155 (9)	0.000	0.0018 (8)	0.000
N1	0.0109 (13)	0.0317 (14)	0.0125 (11)	0.000	0.0003 (10)	0.000

C2	0.0129 (13)	0.0185 (14)	0.0113 (13)	0.000	-0.0021 (10)	0.000
S1	0.0149 (4)	0.0307 (4)	0.0121 (3)	0.000	0.0020 (3)	0.000
N2	0.0124 (12)	0.0196 (12)	0.0110 (11)	0.000	-0.0008 (9)	0.000
C4	0.0134 (13)	0.0108 (13)	0.0146 (13)	0.000	-0.0025 (10)	0.000
C5	0.0183 (14)	0.0129 (13)	0.0128 (13)	0.000	-0.0007 (11)	0.000
C11	0.0149 (4)	0.0262 (4)	0.0132 (3)	0.000	0.0020 (2)	0.000
C6	0.0128 (14)	0.0169 (14)	0.0209 (14)	0.000	0.0010 (11)	0.000
C7	0.0190 (15)	0.0148 (14)	0.0210 (14)	0.000	-0.0057 (12)	0.000
C8	0.0213 (15)	0.0150 (14)	0.0139 (13)	0.000	-0.0018 (11)	0.000
N3	0.0258 (14)	0.0213 (13)	0.0142 (12)	0.000	-0.0011 (10)	0.000
O2	0.0284 (12)	0.0391 (13)	0.0182 (10)	0.000	-0.0114 (9)	0.000
O3	0.0266 (12)	0.0527 (15)	0.0157 (10)	0.000	0.0031 (9)	0.000
C9	0.0165 (14)	0.0122 (13)	0.0154 (13)	0.000	-0.0002 (11)	0.000
C10	0.0147 (14)	0.0258 (15)	0.0104 (13)	0.000	-0.0018 (11)	0.000
C11	0.0193 (17)	0.062 (2)	0.0115 (14)	0.000	-0.0013 (13)	0.000
C12	0.0222 (11)	0.0220 (11)	0.0245 (10)	0.0000 (9)	-0.0078 (8)	-0.0021 (9)

Geometric parameters (Å, °)

C1—O1	1.221 (3)	C7—C8	1.387 (4)
C1—N1	1.392 (3)	C7—H7	0.9500
C1—C10	1.533 (4)	C8—C9	1.380 (4)
N1—C2	1.401 (3)	C8—N3	1.485 (3)
N1—H1N	0.80 (4)	N3—O2	1.226 (3)
C2—N2	1.349 (3)	N3—O3	1.229 (3)
C2—S1	1.667 (3)	C9—H9	0.9500
N2—C4	1.414 (3)	C10—C11	1.526 (4)
N2—H2N	0.97 (3)	C10—C12	1.533 (3)
C4—C9	1.402 (3)	C10—C12 ⁱ	1.533 (3)
C4—C5	1.405 (4)	C11—H11A	0.91 (4)
C5—C6	1.389 (4)	C11—H11B	0.95 (2)
C5—C11	1.740 (3)	C12—H12A	0.9800
C6—C7	1.386 (4)	C12—H12B	0.9800
C6—H6	0.9500	C12—H12C	0.9800
O1—C1—N1	121.1 (2)	C9—C8—C7	123.9 (2)
O1—C1—C10	124.9 (2)	C9—C8—N3	117.9 (2)
N1—C1—C10	113.9 (2)	C7—C8—N3	118.2 (2)
C1—N1—C2	130.6 (2)	O2—N3—O3	124.3 (2)
C1—N1—H1N	116 (3)	O2—N3—C8	117.9 (2)
C2—N1—H1N	113 (3)	O3—N3—C8	117.8 (2)
N2—C2—N1	113.6 (2)	C8—C9—C4	118.8 (2)
N2—C2—S1	129.4 (2)	C8—C9—H9	120.6
N1—C2—S1	117.0 (2)	C4—C9—H9	120.6
C2—N2—C4	130.8 (2)	C11—C10—C12	109.35 (14)
C2—N2—H2N	113.7 (19)	C11—C10—C12 ⁱ	109.35 (14)
C4—N2—H2N	115.5 (19)	C12—C10—C12 ⁱ	111.0 (2)
C9—C4—C5	117.6 (2)	C11—C10—C1	108.6 (2)

C9—C4—N2	124.9 (2)	C12—C10—C1	109.25 (14)
C5—C4—N2	117.5 (2)	C12 ⁱ —C10—C1	109.25 (14)
C6—C5—C4	122.3 (2)	C10—C11—H11A	107 (2)
C6—C5—C11	118.0 (2)	C10—C11—H11B	111.9 (14)
C4—C5—C11	119.7 (2)	H11A—C11—H11B	108.5 (18)
C7—C6—C5	119.9 (2)	C10—C12—H12A	109.5
C7—C6—H6	120.0	C10—C12—H12B	109.5
C5—C6—H6	120.0	H12A—C12—H12B	109.5
C6—C7—C8	117.4 (2)	C10—C12—H12C	109.5
C6—C7—H7	121.3	H12A—C12—H12C	109.5
C8—C7—H7	121.3	H12B—C12—H12C	109.5
O1—C1—N1—C2	0.0	C6—C7—C8—N3	180.0
C10—C1—N1—C2	180.0	C9—C8—N3—O2	180.0
C1—N1—C2—N2	0.0	C7—C8—N3—O2	0.000 (1)
C1—N1—C2—S1	180.0	C9—C8—N3—O3	0.000 (1)
N1—C2—N2—C4	180.0	C7—C8—N3—O3	180.0
S1—C2—N2—C4	0.000 (1)	C7—C8—C9—C4	0.000 (1)
C2—N2—C4—C9	0.000 (1)	N3—C8—C9—C4	180.0
C2—N2—C4—C5	180.0	C5—C4—C9—C8	0.000 (1)
C9—C4—C5—C6	0.0	N2—C4—C9—C8	180.0
N2—C4—C5—C6	180.0	O1—C1—C10—C11	0.0
C9—C4—C5—C11	180.0	N1—C1—C10—C11	180.0
N2—C4—C5—C11	0.0	O1—C1—C10—C12	119.21 (15)
C4—C5—C6—C7	0.000 (1)	N1—C1—C10—C12	-60.79 (15)
C11—C5—C6—C7	180.0	O1—C1—C10—C12 ⁱ	-119.21 (15)
C5—C6—C7—C8	0.000 (1)	N1—C1—C10—C12 ⁱ	60.79 (15)
C6—C7—C8—C9	0.000 (1)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C9—H9 \cdots S1	0.95	2.51	3.197 (3)	130
N2—H2N \cdots O1	0.97 (3)	1.82 (3)	2.653 (3)	141 (3)