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1,1′-(Propane-1,3-diyl)bis[3-(4-chlorophenyl)-thiourea]

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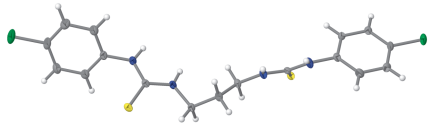
Keywords: crystal structure; thiocarbamide; thiourea derivative; N—H···S hydrogen-bonding.

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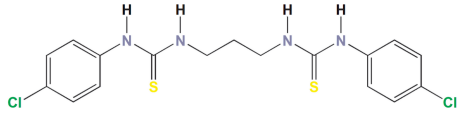
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{17}H_{18}C_{l2}N_4S_2$, crystallizes in the monoclinic space group *I*2/*a* with one molecule in the asymmetric unit. In the molecule, two 1-(4-chlorophenyl)thiourea entities are bridged by a propyl fragment. The thiourea entities are inclined relative to the propyl group in different ways, as shown by the C—C—C—N torsion angles of −71.23 (13) and −179.50 (10)°. In the crystal, N—H···S hydrogen bonds lead to the formation of supramolecular layers parallel to (001).

3D view



Chemical scheme



Structure description

The thiourea moiety is an important pharmacophore for developing new drug prototypes with biological activities including anti-inflammatory, anticancer, antifungal properties (Ölmez & Waseer, 2020; Aguiar *et al.*, 2011; Keche & Kamble, 2014; Abbas *et al.*, 2020). A recent study reported the antimycobactarial and anti-inflammatory activities of thiourea derivatives in the treatment for severe pulmonary tuberculosis (Calixto *et al.*, 2022). Taking into account the presence of a chlorophenyl group in some antimicrobial compounds, we prepared the title thiourea derivative, $C_{17}H_{18}C_{l2}N_4S_2$, and report here its crystal and molecular structure.

The asymmetric unit comprises one molecule (Fig. 1). This consists of two 1-(4-chlorophenyl)thiourea entities bridged by a propyl fragment. The arrangement of the thiourea fragments relative to the propyl fragment is markedly different, as can be seen from the torsion angles of N2—C8—C9—C10 = −71.23 (13)° and N3—C10—C9—C8 = −179.50 (10)°. The dihedral angles between the thiourea fragments and the attached phenyl ring are virtually identical [61.91 (6)° for thiourea group containing S2 and the

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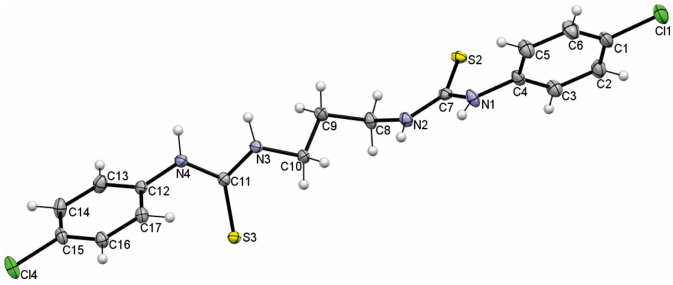


Figure 1
Molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

C1–C6 ring; 61.97 (6)° for S3-thiourea group and the C12–C17 ring]; the thiourea fragments are inclined to each other by a dihedral angle of 71.37 (6)°, and the phenyl rings by 66.91 (6)°.

Two adjacent molecules form a centrosymmetric dimer (Fig. 2) *via* pairwise N—H···S hydrogen bonds (entry #3 in Table 1) with an $R_2^2(16)$ graph-set motif (Etter *et al.*, 1990). These dimers are further connected through somewhat weaker hydrogen bonds (entries 1 and 2 in Table 1), resulting

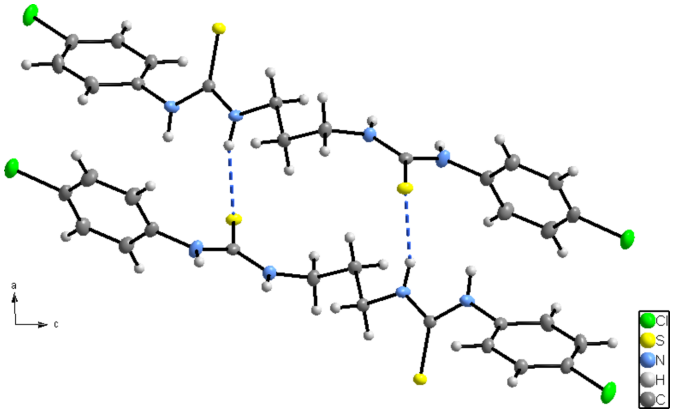


Figure 2
Formation of a centrosymmetric N—H···S hydrogen-bonded dimer with graph-set motif $R_2^2(16)$; hydrogen bonds (entry 3 in Table 1) are shown as blue dashed lines.

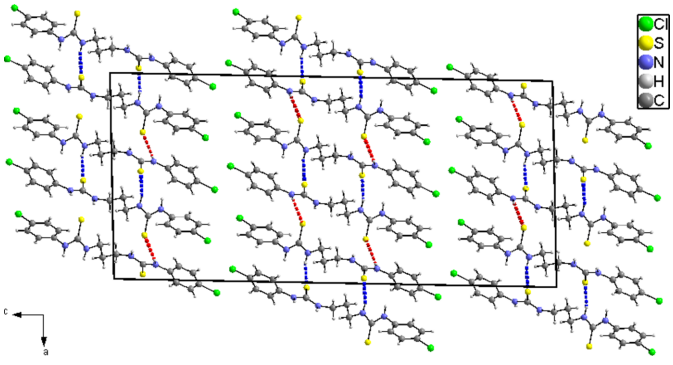


Figure 3
The packing of molecules in the crystal in a projection along [010]. N—H···S hydrogen-bonding interactions are shown as blue dashed lines (entry 3 in Table 1) and red dashed lines (entry 2 in Table 1).

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···S2^{i}	0.88	2.89	3.4950 (11)	128
N2—H2···S3^{ii}	0.88	2.70	3.5386 (10)	161
N3—H3···S2^{iii}	0.88	2.51	3.2827 (10)	147

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}Cl_2N_4S_2$
M_r	413.37
Crystal system, space group	Monoclinic, *I*2/*a*
Temperature (K)	100
a, *b*, *c* (Å)	17.7563 (2), 5.4972 (1), 38.2124 (5)
β (°)	92.168 (1)
V (Å^3)	3727.24 (9)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.58
Crystal size (mm)	0.22 × 0.21 × 0.05
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix-Arc 100
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2022)
T_{min}, T_{max}	0.906, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	54093, 5080, 4601
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.710
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.029, 0.076, 1.03
No. of reflections	5080
No. of parameters	226
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.35

Computer programs: *CrysAlis PRO* (Rigaku OD, 2022), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

in sheets propagating parallel to (001), Fig. 3. The fourth NH group (N4—H4) does not participate in hydrogen bonding.

Synthesis and crystallization

A 3 mmol sample of 4-chlorophenyl isothiocyanate was dissolved in 20 ml of ethanol. This solution was added to a 250 ml flask containing 1,2 diaminopropane (3 mmol). The resulting mixture was stirred at room temperature for one h producing a clear solution. Slow evaporation over the course of weeks produced colourless single-crystals suitable for X-ray diffraction studies.

Refinement

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

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full crystallographic data

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Crystal data

$C_{17}H_{18}Cl_2N_4S_2$
M_r = 413.37
Monoclinic, *I*2/*a*
a = 17.7563 (2) Å
b = 5.4972 (1) Å
c = 38.2124 (5) Å
β = 92.168 (1)°
V = 3727.24 (9) Å^3
Z = 8
F(000) = 1712
D_x = 1.473 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 37150 reflections
θ = 5.4–30.3°
μ = 0.58 mm^{-1}
T = 100 K
Plate, colourless
0.22 × 0.21 × 0.05 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix-Arc 100 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2022)
T_{min} = 0.906, T_{max} = 1.000
54093 measured reflections
5080 independent reflections
4601 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 30.3°, θ_{min} = 5.3°
h = −22→24
k = −7→7
l = −53→53

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.03
5080 reflections
226 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 4.1233P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 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. N-bound hydrogen atoms were discernible from difference-Fourier maps and were modelled with a fixed N—H distance of 0.88 Å and U_{iso}(H) = 1.2U_{eq}(N).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.44228 (2)	1.28574 (8)	0.73158 (2)	0.03525 (10)
Cl4	0.80672 (2)	−0.08518 (7)	0.28692 (2)	0.03111 (9)
S2	0.52537 (2)	1.48529 (5)	0.56514 (2)	0.01720 (7)
S3	0.78472 (2)	0.62155 (5)	0.42899 (2)	0.01515 (7)
N1	0.57320 (6)	1.06881 (19)	0.59471 (3)	0.0203 (2)
H1	0.594183	0.924784	0.592614	0.024*
N2	0.61224 (6)	1.13321 (18)	0.53974 (3)	0.01702 (19)
H2	0.634429	0.990842	0.542284	0.020*
N3	0.64312 (5)	0.76112 (19)	0.43933 (3)	0.0183 (2)
H3	0.594918	0.753224	0.433186	0.022*
N4	0.65752 (6)	0.5310 (2)	0.39102 (3)	0.0189 (2)
H4	0.608792	0.553998	0.387461	0.023*
C1	0.48211 (7)	1.2199 (3)	0.69173 (3)	0.0248 (3)
C2	0.53671 (8)	1.3750 (3)	0.67922 (3)	0.0255 (3)
H2A	0.553131	1.512301	0.692525	0.031*
C3	0.56700 (7)	1.3262 (2)	0.64691 (3)	0.0230 (2)
H3A	0.604765	1.429330	0.638078	0.028*
C4	0.54168 (7)	1.1251 (2)	0.62754 (3)	0.0192 (2)
C5	0.48772 (8)	0.9711 (3)	0.64054 (4)	0.0259 (3)
H5	0.471032	0.833825	0.627278	0.031*
C6	0.45787 (8)	1.0178 (3)	0.67314 (4)	0.0292 (3)
H6	0.421353	0.911746	0.682391	0.035*
C7	0.57360 (6)	1.2175 (2)	0.56657 (3)	0.0156 (2)
C8	0.62026 (7)	1.2604 (2)	0.50650 (3)	0.0190 (2)
H8A	0.672323	1.323510	0.505360	0.023*
H8B	0.585453	1.401093	0.505448	0.023*
C9	0.60351 (7)	1.0963 (2)	0.47508 (3)	0.0189 (2)
H9A	0.554710	1.013312	0.478154	0.023*
H9B	0.598473	1.197759	0.453719	0.023*
C10	0.66419 (7)	0.9056 (2)	0.46999 (3)	0.0168 (2)
H10A	0.713343	0.985770	0.466688	0.020*
H10B	0.669014	0.799749	0.490918	0.020*
C11	0.69113 (6)	0.6393 (2)	0.41971 (3)	0.0144 (2)
C12	0.69487 (6)	0.3836 (2)	0.36636 (3)	0.0163 (2)
C13	0.69330 (8)	0.4534 (2)	0.33133 (3)	0.0221 (2)
H13	0.669108	0.600518	0.324295	0.027*
C14	0.72715 (8)	0.3078 (2)	0.30660 (3)	0.0237 (3)
H14	0.725888	0.353845	0.282618	0.028*
C15	0.76259 (7)	0.0955 (2)	0.31740 (3)	0.0202 (2)
C16	0.76456 (7)	0.0233 (2)	0.35231 (3)	0.0188 (2)
H16	0.789057	−0.123378	0.359314	0.023*
C17	0.73028 (7)	0.1685 (2)	0.37677 (3)	0.0174 (2)
H17	0.730993	0.120824	0.400674	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.03533 (19)	0.0516 (2)	0.01934 (15)	0.01032 (16)	0.00848 (12)	−0.00351 (14)
Cl4	0.0425 (2)	0.03006 (17)	0.02166 (15)	0.00403 (14)	0.01338 (13)	−0.00732 (12)
S2	0.01332 (13)	0.01440 (13)	0.02396 (14)	0.00229 (9)	0.00182 (10)	−0.00305 (10)
S3	0.01252 (13)	0.01588 (13)	0.01699 (13)	0.00161 (9)	−0.00012 (9)	−0.00183 (10)
N1	0.0269 (5)	0.0147 (5)	0.0196 (5)	0.0057 (4)	0.0073 (4)	−0.0015 (4)
N2	0.0194 (5)	0.0140 (4)	0.0178 (4)	0.0039 (4)	0.0023 (4)	−0.0024 (4)
N3	0.0123 (4)	0.0223 (5)	0.0202 (5)	0.0002 (4)	0.0007 (3)	−0.0079 (4)
N4	0.0137 (4)	0.0220 (5)	0.0207 (5)	0.0027 (4)	−0.0018 (4)	−0.0083 (4)
C1	0.0244 (6)	0.0327 (7)	0.0176 (5)	0.0095 (5)	0.0048 (4)	−0.0019 (5)
C2	0.0306 (7)	0.0247 (6)	0.0212 (6)	0.0031 (5)	0.0012 (5)	−0.0062 (5)
C3	0.0250 (6)	0.0213 (6)	0.0229 (6)	−0.0005 (5)	0.0049 (5)	−0.0024 (5)
C4	0.0210 (6)	0.0182 (5)	0.0187 (5)	0.0054 (4)	0.0047 (4)	−0.0016 (4)
C5	0.0293 (7)	0.0236 (6)	0.0252 (6)	−0.0032 (5)	0.0071 (5)	−0.0050 (5)
C6	0.0284 (7)	0.0320 (7)	0.0280 (7)	−0.0038 (6)	0.0103 (5)	−0.0009 (6)
C7	0.0124 (5)	0.0149 (5)	0.0194 (5)	−0.0009 (4)	0.0003 (4)	−0.0039 (4)
C8	0.0243 (6)	0.0160 (5)	0.0168 (5)	0.0024 (4)	0.0028 (4)	−0.0023 (4)
C9	0.0192 (5)	0.0195 (6)	0.0179 (5)	0.0052 (4)	0.0005 (4)	−0.0034 (4)
C10	0.0160 (5)	0.0179 (5)	0.0165 (5)	0.0025 (4)	0.0006 (4)	−0.0047 (4)
C11	0.0154 (5)	0.0122 (5)	0.0155 (5)	−0.0004 (4)	0.0014 (4)	−0.0007 (4)
C12	0.0153 (5)	0.0166 (5)	0.0168 (5)	−0.0005 (4)	−0.0001 (4)	−0.0046 (4)
C13	0.0289 (6)	0.0181 (6)	0.0189 (5)	0.0029 (5)	−0.0040 (5)	−0.0010 (5)
C14	0.0349 (7)	0.0223 (6)	0.0139 (5)	−0.0008 (5)	0.0004 (5)	0.0001 (5)
C15	0.0246 (6)	0.0203 (6)	0.0162 (5)	−0.0016 (5)	0.0058 (4)	−0.0054 (4)
C16	0.0222 (6)	0.0165 (5)	0.0178 (5)	0.0016 (4)	0.0024 (4)	−0.0015 (4)
C17	0.0216 (5)	0.0165 (5)	0.0144 (5)	−0.0011 (4)	0.0023 (4)	−0.0011 (4)

Geometric parameters (Å, º)

Cl1—C1	1.7410 (12)	C4—C5	1.3847 (18)
Cl4—C15	1.7396 (12)	C5—H5	0.9500
S2—C7	1.7029 (12)	C5—C6	1.3961 (18)
S3—C11	1.6889 (11)	C6—H6	0.9500
N1—H1	0.8800	C8—H8A	0.9900
N1—C4	1.4269 (15)	C8—H8B	0.9900
N1—C7	1.3510 (16)	C8—C9	1.5222 (16)
N2—H2	0.8800	C9—H9A	0.9900
N2—C7	1.3380 (14)	C9—H9B	0.9900
N2—C8	1.4613 (15)	C9—C10	1.5210 (16)
N3—H3	0.8800	C10—H10A	0.9900
N3—C10	1.4529 (14)	C10—H10B	0.9900
N3—C11	1.3363 (15)	C12—C13	1.3916 (17)
N4—H4	0.8800	C12—C17	1.3904 (17)
N4—C11	1.3647 (14)	C13—H13	0.9500
N4—C12	1.4252 (14)	C13—C14	1.3921 (18)
C1—C2	1.389 (2)	C14—H14	0.9500

C1—C6	1.379 (2)	C14—C15	1.3817 (18)
C2—H2A	0.9500	C15—C16	1.3912 (16)
C2—C3	1.3910 (17)	C16—H16	0.9500
C3—H3A	0.9500	C16—C17	1.3868 (16)
C3—C4	1.3950 (18)	C17—H17	0.9500

C4—N1—H1	117.2	H8A—C8—H8B	107.9
C7—N1—H1	117.2	C9—C8—H8A	109.1
C7—N1—C4	125.63 (10)	C9—C8—H8B	109.1
C7—N2—H2	117.6	C8—C9—H9A	109.0
C7—N2—C8	124.76 (10)	C8—C9—H9B	109.0
C8—N2—H2	117.6	H9A—C9—H9B	107.8
C10—N3—H3	117.4	C10—C9—C8	113.01 (10)
C11—N3—H3	117.4	C10—C9—H9A	109.0
C11—N3—C10	125.19 (10)	C10—C9—H9B	109.0
C11—N4—H4	117.3	N3—C10—C9	108.53 (9)
C11—N4—C12	125.37 (10)	N3—C10—H10A	110.0
C12—N4—H4	117.3	N3—C10—H10B	110.0
C2—C1—Cl1	119.04 (11)	C9—C10—H10A	110.0
C6—C1—Cl1	119.27 (11)	C9—C10—H10B	110.0
C6—C1—C2	121.68 (12)	H10A—C10—H10B	108.4
C1—C2—H2A	120.5	N3—C11—S3	123.67 (9)
C1—C2—C3	119.04 (12)	N3—C11—N4	113.61 (10)
C3—C2—H2A	120.5	N4—C11—S3	122.71 (9)
C2—C3—H3A	120.1	C13—C12—N4	119.11 (11)
C2—C3—C4	119.73 (12)	C17—C12—N4	120.73 (10)
C4—C3—H3A	120.1	C17—C12—C13	120.12 (11)
C3—C4—N1	120.61 (11)	C12—C13—H13	120.0
C5—C4—N1	118.83 (11)	C12—C13—C14	120.09 (12)
C5—C4—C3	120.51 (11)	C14—C13—H13	120.0
C4—C5—H5	120.0	C13—C14—H14	120.5
C4—C5—C6	119.91 (13)	C15—C14—C13	119.09 (11)
C6—C5—H5	120.0	C15—C14—H14	120.5
C1—C6—C5	119.10 (13)	C14—C15—Cl4	119.60 (9)
C1—C6—H6	120.5	C14—C15—C16	121.47 (11)
C5—C6—H6	120.5	C16—C15—Cl4	118.93 (10)
N1—C7—S2	122.06 (9)	C15—C16—H16	120.4
N2—C7—S2	123.13 (9)	C17—C16—C15	119.11 (11)
N2—C7—N1	114.76 (10)	C17—C16—H16	120.4
N2—C8—H8A	109.1	C12—C17—H17	119.9
N2—C8—H8B	109.1	C16—C17—C12	120.13 (11)
N2—C8—C9	112.30 (10)	C16—C17—H17	119.9

Cl1—C1—C2—C3	−178.19 (10)	C7—N2—C8—C9	−131.43 (12)
Cl1—C1—C6—C5	177.41 (11)	C8—N2—C7—S2	2.01 (16)
Cl4—C15—C16—C17	179.18 (9)	C8—N2—C7—N1	179.55 (11)
N1—C4—C5—C6	177.86 (13)	C8—C9—C10—N3	−179.50 (10)
N2—C8—C9—C10	−71.23 (13)	C10—N3—C11—S3	3.56 (17)

N4—C12—C13—C14	−177.76 (12)	C10—N3—C11—N4	−175.89 (11)
N4—C12—C17—C16	178.16 (11)	C11—N3—C10—C9	155.32 (11)
C1—C2—C3—C4	0.7 (2)	C11—N4—C12—C13	−120.63 (13)
C2—C1—C6—C5	−1.5 (2)	C11—N4—C12—C17	61.58 (17)
C2—C3—C4—N1	−178.60 (12)	C12—N4—C11—S3	2.69 (17)
C2—C3—C4—C5	−1.3 (2)	C12—N4—C11—N3	−177.84 (11)
C3—C4—C5—C6	0.5 (2)	C12—C13—C14—C15	−0.5 (2)
C4—N1—C7—S2	−8.03 (17)	C13—C12—C17—C16	0.38 (18)
C4—N1—C7—N2	174.40 (11)	C13—C14—C15—Cl4	−178.75 (10)
C4—C5—C6—C1	0.9 (2)	C13—C14—C15—C16	0.6 (2)
C6—C1—C2—C3	0.7 (2)	C14—C15—C16—C17	−0.15 (19)
C7—N1—C4—C3	−58.55 (18)	C15—C16—C17—C12	−0.33 (18)
C7—N1—C4—C5	124.08 (14)	C17—C12—C13—C14	0.05 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···S2^{i}	0.88	2.89	3.4950 (11)	128
N2—H2···S3^{ii}	0.88	2.70	3.5386 (10)	161
N3—H3···S2^{iii}	0.88	2.51	3.2827 (10)	147

Symmetry codes: (i) x, $y-1$, z; (ii) $-x+3/2$, y, $-z+1$; (iii) $-x+1$, $-y+2$, $-z+1$.