Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-[(*E*)-2,6-Dichlorobenzylideneamino]-3-{1-[4-(2-methylpropyl)phenyl]ethyl}-1*H*-1,2,4-triazole-5(4*H*)-thione

Hoong-Kun Fun,[a]* Suchada Chantrapromma,[b]‡ K. V. Sujith,[c] P. S. Patil,[d] B. Kalluraya,[c] A. Muralidharan[e] and S. M. Dharmaprakash[d]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Crystal Materials Research Unit, Department of Chemistry, Faculty of Science, Prince of Songkla University, Hat-Yai, Songkhla 90112, Thailand, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri, Mangalore 574 199, India, [d]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India, and [e]Department of Chemistry, Nehru Arts & Science College, Kanhangad, Kerala 671 328, India
Correspondence e-mail: hkfun@usm.my

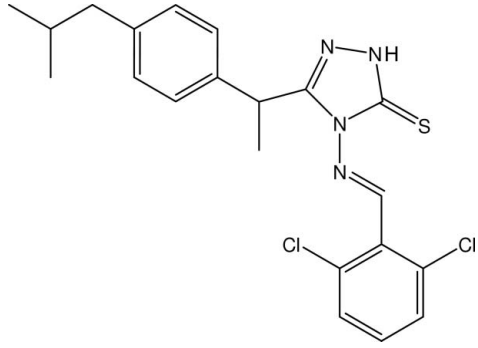
Received 7 July 2008; accepted 9 July 2008

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.136; data-to-parameter ratio = 23.6.

In the title Schiff base compound, $C_{21}H_{22}Cl_2N_4S$, the triazole ring makes dihedral angles of 2.15 (11) and 87.48 (11)° with the 2,6-dichlorophenyl and methylpropylphenyl rings, respectively. Weak intramolecular C—H···S and C—H···Cl interactions generate S(6) and S(5) ring motifs, respectively. In the crystal structure, centrosymmetrically related molecules are linked into dimers by N—H···S hydrogen bonds. These dimers are arranged into sheets parallel to the *ab* plane and are stacked along the *c* axis. C—H···π interactions involving the methylpropylphenyl ring and π–π interactions involving the dichlorophenyl ring [centroid–centroid distance = 3.5865 (3) Å] are also observed.

Related literature

For related literature on hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For related structures, see: Fun *et al.* (2008*a*,*b*). For background to the activities and applications of 1,2,4-triazole derivatives, see: Almasirad *et al.* (2004); Al-Soud *et al.* (2003); Amir & Shikha (2004); Holla *et al.* (2003); Kawashima *et al.* (1987); Palaska *et al.* (2002); Walczak *et al.* (2004); Zitouni *et al.* (2005).



Experimental

Crystal data

$C_{21}H_{22}Cl_2N_4S$
M_r = 433.40
Triclinic, $P\overline{1}$
a = 8.6190 (2) Å
b = 9.4441 (2) Å
c = 14.4244 (4) Å
α = 104.669 (2)°
β = 95.492 (2)°
γ = 110.418 (1)°
V = 1042.33 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 100.0 (1) K
0.29 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.887, T_{max} = 0.934
19865 measured reflections
6032 independent reflections
4139 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.00
6032 reflections
256 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···S1^{i}	0.86	2.44	3.2849 (19)	169
C10—H10*A*···Cl2	0.93	2.62	2.978 (2)	104
C10—H10*A*···S1	0.93	2.52	3.2066 (19)	131
C15—H15*A*···*Cg*1^{ii}	0.93	2.94	3.793 (3)	154

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

KVS, BK and AM are grateful to Kerala State Council for Science Technology and Environment, Thiruvananthapuram, for financial assistance. The authors also thank Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

‡ Additional correspondence author, e-mail: suchada.c@psu.ac.th.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2627).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.

Almasirad, A., Tabatabai, S. A., Faizi, M., Kebriaeezadeh, A., Mehrabi, N., Dalvandi, A. & Shafiee, A. (2004). *Bioorg. Med. Chem. Lett.* **14**, 6057–6059.

Al-Soud, Y. A., Al-Masoudi, N. A. & Ferwanah, A. R. S. (2003). *Bioorg. Med. Chem.* **11**, 1701–1708.

Amir, M. & Shikha, K. (2004). *Eur. J. Med. Chem.* **39**, 535–545.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Fun, H.-K., Jebas, S. R., Razak, I. A., Sujith, K. V., Patil, P. S., Kalluraya, B. & Dharmaprakash, S. M. (2008*a*). *Acta Cryst.* E**64**, o1076–o1077.

Fun, H.-K., Jebas, S. R., Sujith, K. V., Patil, P. S., Kalluraya, B. & Dharmaprakash, S. M. (2008*b*). *Acta Cryst.* E**64**, o1001–o1002.

Holla, B. S., Veerendra, B., Shivananda, M. K. & Poojary, B. (2003). *Eur. J. Med. Chem.* **38**, 759–767.

Kawashima, Y., Ishikawa, H., Kida, S., Tanaka, T. & Masuda, T. (1987). *Chem Abstr.* **106**, 138475x.

Palaska, E., Sahin, G., Kelicen, P., Durlu, N. T. & Altinok, G. (2002). *Il Farmaco*, **57**, 101–107.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Walczak, K., Gondela, A. & Suwin'ski, J. (2004). *Eur. J. Med. Chem.* **39**, 849–853.

Zitouni, G. T., Kaplancíklí, Z. A., Yíldíz, M. T., Chevallet, P. & Kaya, D. (2005). *Eur. J. Med. Chem.* **40**, 607–613.

supporting information

Acta Cryst. (2008). E**64**, o1503–o1504 [doi:10.1107/S1600536808021272]

4-[(*E*)-2,6-Dichlorobenzylideneamino]-3-{1-[4-(2-methylpropyl)phenyl]-ethyl}-1*H*-1,2,4-triazole-5(4*H*)-thione

Hoong-Kun Fun, Suchada Chantrapromma, K. V. Sujith, P. S. Patil, B. Kalluraya, A. Muralidharan and S. M. Dharmaprakash

S1. Comment

1,2,4-Triazoles and their derivatives represent an overwhelming and rapid developing field in modern heterocyclic chemistry. A degree of respectability has been bestowed for 1,2,4-triazole derivatives due to their antibacterial, antifungal (Zitouni *et al.*, 2005), antitubercular (Walczak *et al.*, 2004), anticancer (Holla *et al.*, 2003), antitumor (Al-Soud *et al.*, 2003), anticonvulsant (Almasirad *et al.*, 2004), antiinflammatory, and analgesic properties (Amir & Shikha, 2004). Certain 1,2,4-triazoles also find applications in the preparation of photographic plates, polymers, and as analytical agents (Kawashima *et al.*, 1987). Similarly, ibuprofen belongs to the class of Non-Steroidal Anti-Inflammatory Drugs (NSAIDs) with antipyretic, anti-inflammatory and analgesic properties (Palaska *et al.*, 2002). Our earlier studies involved synthesis of heterocyclic compounds which contain in their structures both the ibuprofen and 1,2,4-triazole fragments (Fun *et al.*, 2008*a*,*b*). In this connection and in continuation of our interest in the synthesis of chemically and biologically important heterocycles, we report here the crystal structure of a substituted 1,2,4-triazole Schiff base carrying only the ibuprofen moiety.

In the title Schiff base compound (Fig. 1), the 1,2,4 triazole ring (C8-C9/N1-N3) is planar with a maximum deviation of 0.009 (2) Å for atom N3. The 1,2,4 triazole ring is co-planar with the 2,6-dichlorophenyl (C11-C16) ring [dihedral angle = 2.15 (11)°] but is almost perpendicular to the methylpropylphenyl (C1-C6) ring with a dihedral angle of 87.48 (11)°. The methylidene amino linkage (N4/C10) is slightly twisted from the mean plane of the 1,2,4 triazole ring as indicated by the torsion angle C9–N3–N4–C10 of 26.4 (3)°. Weak C—H···S and C—H···Cl intramolecular interactions generate S(6) and S(5) ring motifs, respectively (Bernstein *et al.*, 1995). The bond distances and angles have normal values (Allen *et al.*, 1987) and are comparable with closely related structures (Fun *et al.*, 2008*a*,*b*).

In the crystal structure, centrosymmetrically related molecules are linked into dimers (Fig. 2) by N—H···S hydrogen bonds (Table 1). These dimers are arranged into sheets parallel to the *ab* plane and these sheets are stacked along the *c* axis (Fig. 3). In addition, the crystal structure is stabilized by C—H···π interactions (Table 1) involving the C1-C6 ring (centroid Cg1) and π-π interaction involving the C11-C16 ring (centroid Cg2) [$Cg_2\cdots Cg_2^{ii}$ = 3.5865 (3) Å, symmetry code: (ii) 1 - *x*, -*y*, -*z*].

S2. Experimental

The title compound was obtained by refluxing 4-amino-5-[1-(4-isobutylphenyl)ethyl]-4*H*-1,2,4-triazole-3-thiol (0.01 mol) and 2,6-dichlorobenzaldehyde (0.01 mol) in ethanol (50 ml) with the addition of 3 drops of concentrated sulfuric acid for 3 h. The solid product obtained was collected by filtration, washed with ethanol and dried. Colourless single crystals suitable for X-ray analysis were obtained from a acetone-*N*,*N*-dimethylformamide (DMF) (1:3 *v*/*v*) solution by

slow evaporation (yield 53%; m.p. 438–440 K)

S3. Refinement

All H atoms were placed in calculated positions (N-H = 0.86 Å and C-H = 0.93-0.98 Å) and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C,N) and 1.5U_{eq}(C_{methyl}). A rotating group model was used for the methyl groups.

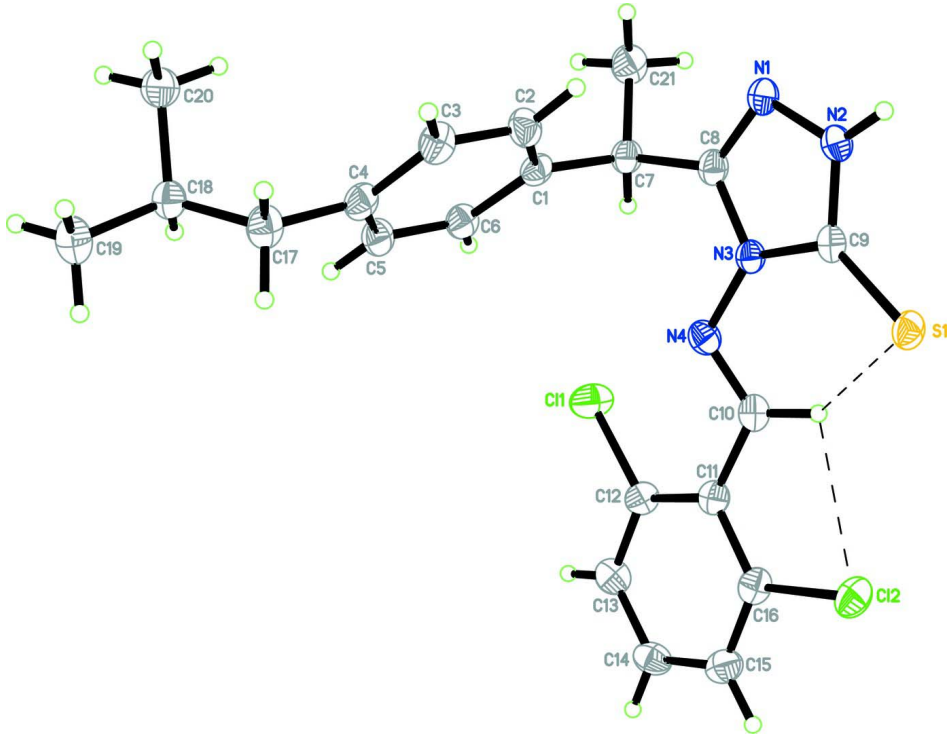


Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Weak C—H···S and C—H···Cl hydrogen bonds are shown as dashed lines.

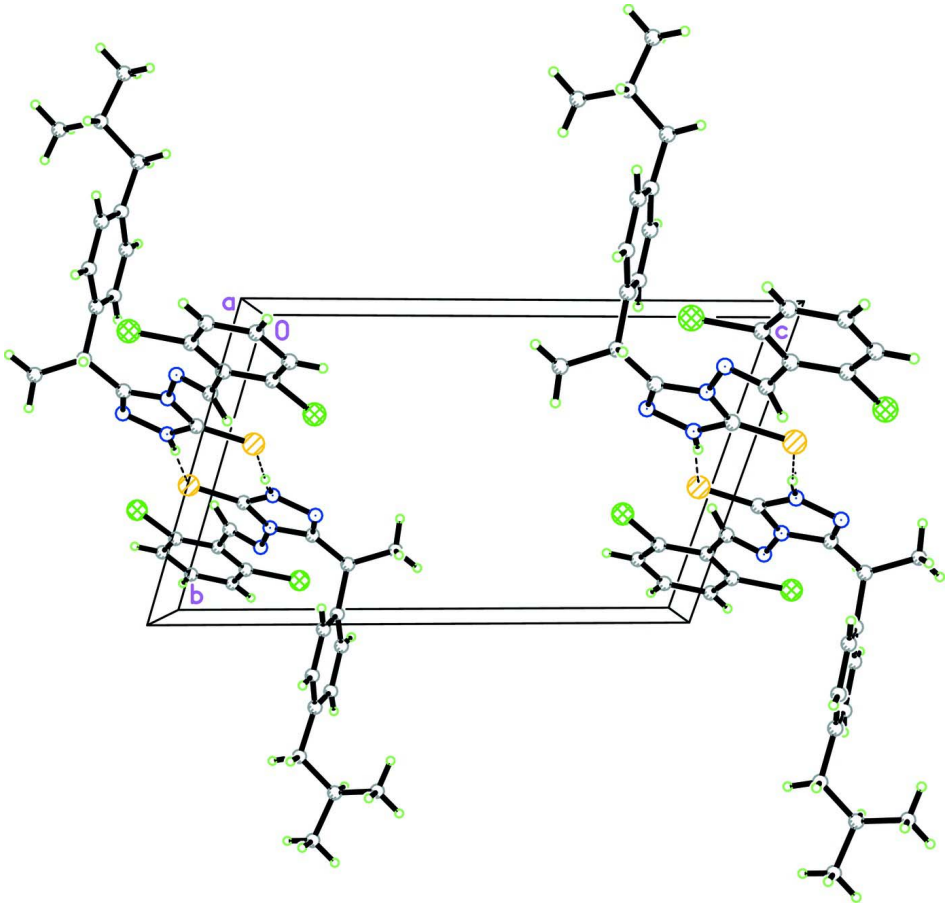


Figure 2

Part of the crystal packing of the title compound, viewed along the *a* axis, showing hydrogen-bonded (dashed lines) dimers.

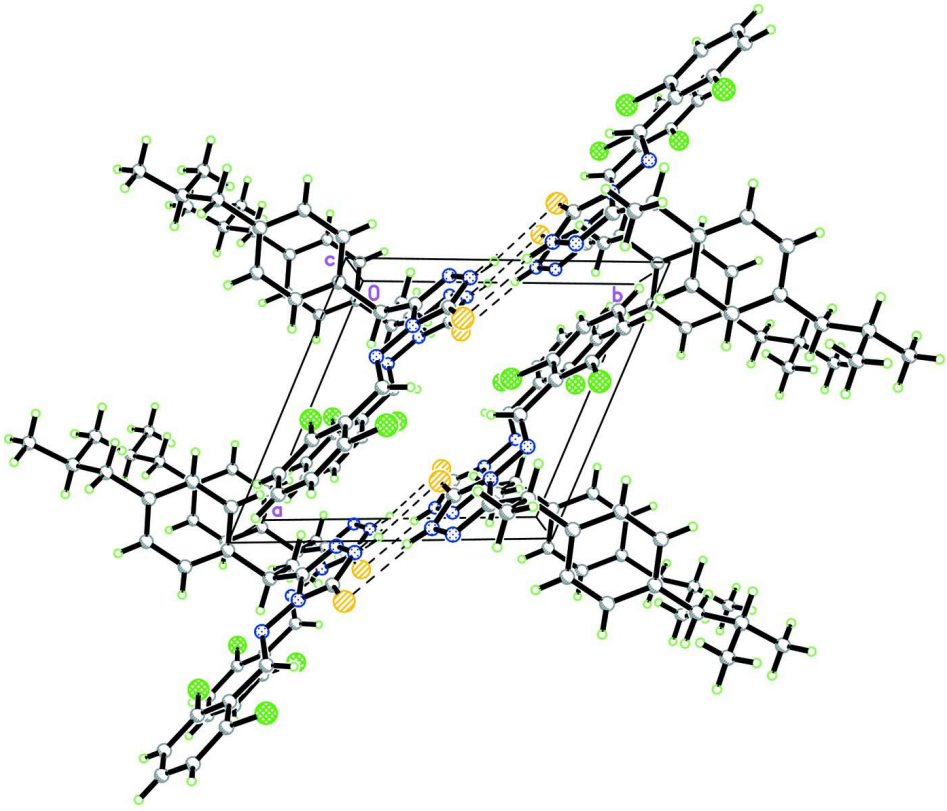


Figure 3

The packing diagram of the title compound, viewed along the *c* axis, showing stacking of the molecular sheets. Hydrogen bonds are shown as dashed lines.

4-[(*E*)-2,6-Dichlorobenzylideneamino]-3-{1-[4-(2- methylpropyl)phenyl]ethyl}-1*H*-1,2,4-triazole-5(4H)-thione

Crystal data

$C_{21}H_{22}Cl_2N_4S$
M_r = 433.40
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.6190 (2) Å
b = 9.4441 (2) Å
c = 14.4244 (4) Å
α = 104.669 (2)°
β = 95.492 (2)°
γ = 110.418 (1)°
V = 1042.33 (5) Å^3
Z = 2
F(000) = 452
D_x = 1.381 Mg m^{-3}
Melting point = 438–440 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6032 reflections
θ = 1.5–30.0°
μ = 0.43 mm^{-1}
T = 100 K
Block, colourless
0.29 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.887, T_{max} = 0.935
19865 measured reflections
6032 independent reflections
4139 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

θ_{max} = 30.0°, θ_{min} = 1.5°
h = −12→12
k = −13→13
l = −20→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.136
S = 1.00
6032 reflections
256 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.
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	0.79027 (6)	−0.43005 (6)	−0.06227 (3)	0.02335 (13)
Cl1	0.43164 (7)	−0.07928 (7)	0.21127 (4)	0.03523 (15)
Cl2	0.41695 (7)	−0.33808 (6)	−0.17537 (4)	0.03136 (14)
N1	0.9611 (2)	−0.3270 (2)	0.21761 (12)	0.0244 (4)
N2	0.9465 (2)	−0.3961 (2)	0.11923 (12)	0.0240 (4)
H2A	1.0037	−0.4511	0.0971	0.029*
N3	0.7738 (2)	−0.28053 (18)	0.12730 (11)	0.0192 (3)
N4	0.6602 (2)	−0.20834 (19)	0.11584 (12)	0.0229 (4)
C1	0.9409 (2)	0.0211 (2)	0.32320 (13)	0.0218 (4)
C2	1.1052 (3)	0.0657 (2)	0.30759 (15)	0.0259 (4)
H2B	1.1515	−0.0105	0.2915	0.031*
C3	1.2013 (3)	0.2223 (2)	0.31568 (15)	0.0266 (4)
H3A	1.3109	0.2492	0.3046	0.032*
C4	1.1366 (3)	0.3403 (2)	0.34015 (14)	0.0244 (4)
C5	0.9747 (3)	0.2957 (2)	0.35952 (14)	0.0262 (4)
H5A	0.9301	0.3726	0.3786	0.031*
C6	0.8779 (3)	0.1389 (2)	0.35107 (14)	0.0234 (4)
H6A	0.7696	0.1125	0.3642	0.028*
C7	0.8319 (3)	−0.1523 (2)	0.31079 (14)	0.0225 (4)
H7A	0.7131	−0.1651	0.3013	0.027*
C8	0.8563 (2)	−0.2560 (2)	0.22068 (14)	0.0217 (4)
C9	0.8351 (2)	−0.3702 (2)	0.06064 (14)	0.0206 (4)

C10	0.5498 (2)	−0.2695 (2)	0.03633 (14)	0.0223 (4)
H10A	0.5495	−0.3578	−0.0105	0.027*
C11	0.4228 (2)	−0.2036 (2)	0.01691 (14)	0.0215 (4)
C12	0.3619 (3)	−0.1177 (2)	0.08757 (15)	0.0239 (4)
C13	0.2388 (3)	−0.0628 (2)	0.06263 (16)	0.0270 (4)
H13A	0.2011	−0.0054	0.1112	0.032*
C14	0.1729 (3)	−0.0938 (2)	−0.03479 (16)	0.0278 (5)
H14A	0.0906	−0.0570	−0.0516	0.033*
C15	0.2278 (3)	−0.1792 (3)	−0.10761 (16)	0.0284 (5)
H15A	0.1829	−0.2003	−0.1732	0.034*
C16	0.3504 (3)	−0.2325 (2)	−0.08126 (14)	0.0246 (4)
C17	1.2359 (3)	0.5077 (2)	0.34117 (15)	0.0281 (5)
H17A	1.1787	0.5286	0.2881	0.034*
H17B	1.3462	0.5147	0.3281	0.034*
C18	1.2612 (3)	0.6380 (2)	0.43631 (15)	0.0248 (4)
H18A	1.1498	0.6274	0.4512	0.030*
C19	1.3448 (3)	0.8002 (2)	0.42311 (17)	0.0331 (5)
H19A	1.3584	0.8813	0.4826	0.050*
H19B	1.2752	0.8098	0.3709	0.050*
H19C	1.4535	0.8121	0.4075	0.050*
C20	1.3655 (3)	0.6216 (3)	0.52176 (15)	0.0307 (5)
H20A	1.3751	0.7017	0.5808	0.046*
H20B	1.4763	0.6345	0.5092	0.046*
H20C	1.3109	0.5185	0.5289	0.046*
C21	0.8713 (3)	−0.2028 (3)	0.39995 (15)	0.0315 (5)
H21A	0.8010	−0.3124	0.3882	0.047*
H21B	0.8496	−0.1387	0.4564	0.047*
H21C	0.9880	−0.1890	0.4113	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0258 (3)	0.0241 (2)	0.0194 (2)	0.0112 (2)	0.00672 (19)	0.00244 (18)
Cl1	0.0389 (3)	0.0551 (4)	0.0221 (3)	0.0310 (3)	0.0104 (2)	0.0093 (2)
Cl2	0.0362 (3)	0.0338 (3)	0.0213 (3)	0.0135 (2)	0.0063 (2)	0.0036 (2)
N1	0.0296 (9)	0.0241 (8)	0.0190 (8)	0.0132 (7)	0.0055 (7)	0.0016 (7)
N2	0.0272 (9)	0.0240 (8)	0.0228 (8)	0.0152 (7)	0.0061 (7)	0.0030 (7)
N3	0.0210 (8)	0.0184 (7)	0.0182 (8)	0.0081 (6)	0.0061 (6)	0.0043 (6)
N4	0.0241 (8)	0.0230 (8)	0.0247 (9)	0.0120 (7)	0.0080 (7)	0.0072 (7)
C1	0.0245 (10)	0.0248 (10)	0.0144 (9)	0.0095 (8)	0.0034 (7)	0.0036 (7)
C2	0.0280 (10)	0.0235 (10)	0.0270 (11)	0.0134 (8)	0.0080 (8)	0.0033 (8)
C3	0.0245 (10)	0.0280 (10)	0.0245 (10)	0.0090 (8)	0.0086 (8)	0.0037 (8)
C4	0.0299 (10)	0.0252 (10)	0.0159 (9)	0.0108 (8)	0.0050 (8)	0.0023 (8)
C5	0.0293 (10)	0.0250 (10)	0.0242 (10)	0.0140 (8)	0.0062 (8)	0.0020 (8)
C6	0.0245 (10)	0.0261 (10)	0.0205 (9)	0.0124 (8)	0.0072 (8)	0.0037 (8)
C7	0.0251 (10)	0.0229 (9)	0.0195 (9)	0.0103 (8)	0.0064 (8)	0.0042 (7)
C8	0.0249 (10)	0.0194 (9)	0.0199 (9)	0.0075 (8)	0.0069 (7)	0.0051 (7)
C9	0.0227 (9)	0.0165 (8)	0.0212 (9)	0.0067 (7)	0.0071 (7)	0.0039 (7)

C10	0.0216 (9)	0.0203 (9)	0.0237 (10)	0.0066 (8)	0.0081 (8)	0.0054 (7)
C11	0.0192 (9)	0.0203 (9)	0.0235 (10)	0.0049 (7)	0.0062 (8)	0.0072 (7)
C12	0.0228 (10)	0.0270 (10)	0.0223 (10)	0.0093 (8)	0.0068 (8)	0.0082 (8)
C13	0.0225 (10)	0.0300 (11)	0.0323 (11)	0.0125 (8)	0.0106 (8)	0.0113 (9)
C14	0.0219 (10)	0.0300 (11)	0.0356 (12)	0.0107 (9)	0.0062 (9)	0.0158 (9)
C15	0.0274 (10)	0.0296 (11)	0.0255 (11)	0.0074 (9)	0.0028 (8)	0.0103 (8)
C16	0.0246 (10)	0.0244 (10)	0.0226 (10)	0.0065 (8)	0.0079 (8)	0.0064 (8)
C17	0.0349 (12)	0.0259 (10)	0.0224 (10)	0.0104 (9)	0.0104 (9)	0.0060 (8)
C18	0.0267 (10)	0.0220 (10)	0.0241 (10)	0.0086 (8)	0.0062 (8)	0.0053 (8)
C19	0.0390 (13)	0.0245 (10)	0.0335 (12)	0.0102 (10)	0.0105 (10)	0.0070 (9)
C20	0.0353 (12)	0.0306 (11)	0.0264 (11)	0.0164 (9)	0.0049 (9)	0.0046 (9)
C21	0.0416 (13)	0.0319 (11)	0.0234 (11)	0.0159 (10)	0.0103 (9)	0.0088 (9)

Geometric parameters (Å, º)

S1—C9	1.6797 (19)	C10—C11	1.472 (3)
Cl1—C12	1.730 (2)	C10—H10A	0.93
Cl2—C16	1.740 (2)	C11—C12	1.398 (3)
N1—C8	1.297 (2)	C11—C16	1.409 (3)
N1—N2	1.377 (2)	C12—C13	1.389 (3)
N2—C9	1.345 (2)	C13—C14	1.381 (3)
N2—H2A	0.86	C13—H13A	0.93
N3—C8	1.384 (2)	C14—C15	1.382 (3)
N3—C9	1.385 (2)	C14—H14A	0.93
N3—N4	1.394 (2)	C15—C16	1.381 (3)
N4—C10	1.275 (2)	C15—H15A	0.93
C1—C2	1.388 (3)	C17—C18	1.531 (3)
C1—C6	1.390 (3)	C17—H17A	0.97
C1—C7	1.530 (3)	C17—H17B	0.97
C2—C3	1.388 (3)	C18—C19	1.519 (3)
C2—H2B	0.93	C18—C20	1.527 (3)
C3—C4	1.396 (3)	C18—H18A	0.98
C3—H3A	0.93	C19—H19A	0.96
C4—C5	1.388 (3)	C19—H19B	0.96
C4—C17	1.508 (3)	C19—H19C	0.96
C5—C6	1.389 (3)	C20—H20A	0.96
C5—H5A	0.93	C20—H20B	0.96
C6—H6A	0.93	C20—H20C	0.96
C7—C8	1.498 (3)	C21—H21A	0.96
C7—C21	1.529 (3)	C21—H21B	0.96
C7—H7A	0.98	C21—H21C	0.96
C8—N1—N2	104.17 (15)	C13—C12—Cl1	116.33 (16)
C9—N2—N1	114.24 (15)	C11—C12—Cl1	121.52 (16)
C9—N2—H2A	122.9	C14—C13—C12	119.57 (19)
N1—N2—H2A	122.9	C14—C13—H13A	120.2
C8—N3—C9	108.43 (15)	C12—C13—H13A	120.2
C8—N3—N4	119.01 (15)	C13—C14—C15	120.7 (2)

C9—N3—N4	132.41 (16)	C13—C14—H14A	119.6
C10—N4—N3	117.04 (16)	C15—C14—H14A	119.6
C2—C1—C6	117.99 (19)	C16—C15—C14	118.81 (19)
C2—C1—C7	121.30 (17)	C16—C15—H15A	120.6
C6—C1—C7	120.71 (18)	C14—C15—H15A	120.6
C1—C2—C3	121.00 (18)	C15—C16—C11	122.96 (19)
C1—C2—H2B	119.5	C15—C16—Cl2	117.26 (16)
C3—C2—H2B	119.5	C11—C16—Cl2	119.79 (16)
C2—C3—C4	121.3 (2)	C4—C17—C18	115.60 (17)
C2—C3—H3A	119.4	C4—C17—H17A	108.4
C4—C3—H3A	119.4	C18—C17—H17A	108.4
C5—C4—C3	117.32 (19)	C4—C17—H17B	108.4
C5—C4—C17	121.41 (18)	C18—C17—H17B	108.4
C3—C4—C17	121.22 (19)	H17A—C17—H17B	107.4
C4—C5—C6	121.51 (18)	C19—C18—C20	110.68 (17)
C4—C5—H5A	119.2	C19—C18—C17	109.89 (18)
C6—C5—H5A	119.2	C20—C18—C17	111.28 (17)
C5—C6—C1	120.83 (19)	C19—C18—H18A	108.3
C5—C6—H6A	119.6	C20—C18—H18A	108.3
C1—C6—H6A	119.6	C17—C18—H18A	108.3
C8—C7—C21	110.54 (16)	C18—C19—H19A	109.5
C8—C7—C1	108.88 (16)	C18—C19—H19B	109.5
C21—C7—C1	112.70 (16)	H19A—C19—H19B	109.5
C8—C7—H7A	108.2	C18—C19—H19C	109.5
C21—C7—H7A	108.2	H19A—C19—H19C	109.5
C1—C7—H7A	108.2	H19B—C19—H19C	109.5
N1—C8—N3	110.81 (16)	C18—C20—H20A	109.5
N1—C8—C7	126.05 (18)	C18—C20—H20B	109.5
N3—C8—C7	123.04 (17)	H20A—C20—H20B	109.5
N2—C9—N3	102.32 (15)	C18—C20—H20C	109.5
N2—C9—S1	127.33 (15)	H20A—C20—H20C	109.5
N3—C9—S1	130.33 (15)	H20B—C20—H20C	109.5
N4—C10—C11	121.60 (18)	C7—C21—H21A	109.5
N4—C10—H10A	119.2	C7—C21—H21B	109.5
C11—C10—H10A	119.2	H21A—C21—H21B	109.5
C12—C11—C16	115.84 (18)	C7—C21—H21C	109.5
C12—C11—C10	125.92 (18)	H21A—C21—H21C	109.5
C16—C11—C10	118.21 (17)	H21B—C21—H21C	109.5
C13—C12—C11	122.11 (19)		

C8—N1—N2—C9	0.0 (2)	N1—N2—C9—N3	−1.0 (2)
C8—N3—N4—C10	−158.60 (18)	N1—N2—C9—S1	177.52 (14)
C9—N3—N4—C10	26.4 (3)	C8—N3—C9—N2	1.52 (19)
C6—C1—C2—C3	−2.6 (3)	N4—N3—C9—N2	176.87 (18)
C7—C1—C2—C3	177.75 (18)	C8—N3—C9—S1	−176.89 (16)
C1—C2—C3—C4	0.3 (3)	N4—N3—C9—S1	−1.5 (3)
C2—C3—C4—C5	2.3 (3)	N3—N4—C10—C11	179.51 (17)
C2—C3—C4—C17	−175.13 (19)	N4—C10—C11—C12	−26.3 (3)

C3—C4—C5—C6	−2.6 (3)	N4—C10—C11—C16	155.8 (2)
C17—C4—C5—C6	174.83 (19)	C16—C11—C12—C13	−0.6 (3)
C4—C5—C6—C1	0.3 (3)	C10—C11—C12—C13	−178.53 (19)
C2—C1—C6—C5	2.3 (3)	C16—C11—C12—Cl1	177.38 (15)
C7—C1—C6—C5	−178.04 (18)	C10—C11—C12—Cl1	−0.6 (3)
C2—C1—C7—C8	−42.3 (2)	C11—C12—C13—C14	0.3 (3)
C6—C1—C7—C8	138.03 (19)	Cl1—C12—C13—C14	−177.75 (16)
C2—C1—C7—C21	80.7 (2)	C12—C13—C14—C15	0.1 (3)
C6—C1—C7—C21	−98.9 (2)	C13—C14—C15—C16	−0.2 (3)
N2—N1—C8—N3	1.0 (2)	C14—C15—C16—C11	−0.1 (3)
N2—N1—C8—C7	−175.37 (18)	C14—C15—C16—Cl2	−179.50 (16)
C9—N3—C8—N1	−1.7 (2)	C12—C11—C16—C15	0.5 (3)
N4—N3—C8—N1	−177.76 (17)	C10—C11—C16—C15	178.60 (19)
C9—N3—C8—C7	174.84 (17)	C12—C11—C16—Cl2	179.88 (15)
N4—N3—C8—C7	−1.2 (3)	C10—C11—C16—Cl2	−2.0 (2)
C21—C7—C8—N1	−29.1 (3)	C5—C4—C17—C18	56.3 (3)
C1—C7—C8—N1	95.2 (2)	C3—C4—C17—C18	−126.4 (2)
C21—C7—C8—N3	154.92 (18)	C4—C17—C18—C19	−173.51 (18)
C1—C7—C8—N3	−80.8 (2)	C4—C17—C18—C20	63.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···S1^{i}	0.86	2.44	3.2849 (19)	169
C10—H10*A*···Cl2	0.93	2.62	2.978 (2)	104
C10—H10*A*···S1	0.93	2.52	3.2066 (19)	131
C15—H15*A*···*Cg*1^{ii}	0.93	2.94	3.793 (3)	154

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