Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-(1-Adamantyl)-3-(2-fluorophenyl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

Mahmood-ul-Hassan Khan,[a] Shahid Hameed,[a]‡ M. Nawaz Tahir,[b]* Tanveer Hussain Bokhari[c] and Islam Ullah Khan[c]

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, [b]Department of Physics, University of Sargodha, Sargodha, Pakistan, and [c]Department of Chemistry, Government College University, Lahore, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

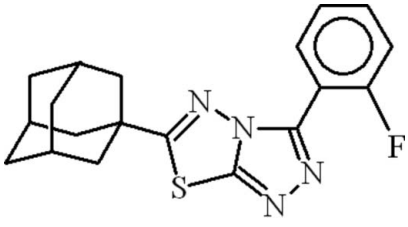
Received 24 May 2009; accepted 24 May 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.136; data-to-parameter ratio = 19.1.

In the title compound, $C_{19}H_{19}FN_4S$, the planes of the 2-fluorophenyl and 1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole ring systems are oriented at a dihedral angle of 48.98 (6)°. In the crystal, weak C—H···S and C—H···π interactions may help to establish the packing and π–π interactions between the centroids of the benzene rings at a distance of 3.8792 (13) Å occur.

Related literature

For a related structure, see: Holm *et al.* (2008). For our previous studies on related compounds, see: Akhtar *et al.* (2007, 2008*a*,*b*). For background to the biological activity of related compounds, see: El-Emam *et al.* (2004); Kadi *et al.* (2007); Zhang *et al.* (2002).



Experimental

Crystal data

$C_{19}H_{19}FN_4S$
M_r = 354.44
Orthorhombic, *Pbca*
a = 13.2684 (9) Å
b = 12.4293 (9) Å
c = 20.2231 (15) Å
V = 3335.1 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 296 K
0.25 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.945, T_{max} = 0.956
22695 measured reflections
4486 independent reflections
3116 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.04
4486 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···S1^{i}	0.97	2.84	3.640 (2)	140
C12—H12···$Cg1^{ii}$	0.98	2.90	3.713 (2)	140
C18—H18B···$Cg1^{iii}$	0.97	2.83	3.787 (3)	170

Symmetry codes: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, y, -z+\frac{1}{2}$. $Cg1$ is the centroid of the S1/C8/N3/N4/C9 ring.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

The authors acknowledge the Higher Education Commission, Islamabad, Pakistan, and Bana International, Karachi, Pakistan, for funding the purchase of the diffractometer and for technical support, respectively.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2984).

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‡ Additional correspondence author for matters regarding the chemistry, e-mail: shameed@qau.edu.pk.

supporting information

Acta Cryst. (2009). E**65**, o1437 [doi:10.1107/S1600536809019692]

6-(1-Adamantyl)-3-(2-fluorophenyl)-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

Mahmood-ul-Hassan Khan, Shahid Hameed, M. Nawaz Tahir, Tanveer Hussain Bokhari and Islam Ullah Khan

S1. Comment

Five membered heterocycles bearing adamantyl moiety are gaining importance due to their promising biological activities (El-Emam *et al.*, 2004; Kadi *et al.*, 2007). On the other hand the condensed heterocyclic systems *e.g.*, triazolo-thiadiazoles exhibit numerous biological activities (Zhang *et al.*, 2002). In continuation of our previous studeis (Akhtar *et al.*, 2007, 2008*a*, 2008*b*), the title compound, (I), (Fig. 1), has been synthesized with the hope that it will possess antiviral and anticancer activity. The crystal structure of (II) 3-(2-Fluorophenyl)-6-(phenoxymethyl)-1,2,4- triazolo(3,4 - b) (1,3,4)thiadiazole (Holm, *et al.*, 2008) has been published which has a common moiety as in (I).

In (I), the ring A (C1—C6) along with F1-atom and two [(C7/N1/N2/C8/N3) & (C8/S1/C9/N4/N3)] fused heterocyclic rings B (C7/N1/N2/C8/S1/C9/N4/N3) are planar and oriented at a dihedral angle of 48.98 (6)°. There exist π—π interaction between the centroids, CgA—CgA^{i} [symmetry code: i = 1 - *x*, -*y*, 1 - *z*], of benzene rings at a distance of 3.8792 (13) Å. In the crystal, the packing is consolidated by H-bonding (Fig 2) and C—H···π interactions (Table 1).

S2. Experimental

A mixture of 4-amino-5-(2-fluorophenyl)-2*H*-1,2,4-triazole-3(4*H*)-thione (0.2 g, 0.56 mmol) and adamantane-1-carboxylic acid (0.10 g, 0.56 mmol) in the presence of $POCl_3$ (5 ml) was refluxed for four hours. The reaction mixture was cooled to room temperature, poured into crushed ice and neutralized using solid potassium carbonate until pH was 8. The precipitated solid was filtered, washed with excess water and recrystallized from chloroform to yield colourless prisms of (I).

S3. Refinement

H-atoms were positioned in calculated positions with C-H = 0.93–0.98 Å and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

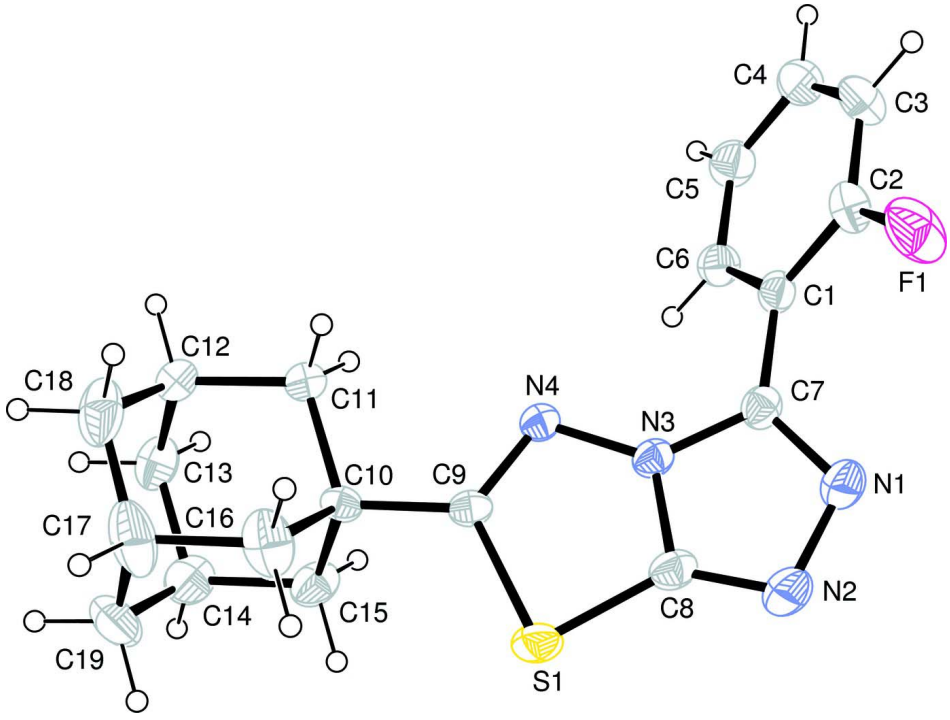

Figure 1

View of (I) with displacement ellipsoids drawn at the 30% probability level. H-atoms are shown by small spheres of arbitrary radius.

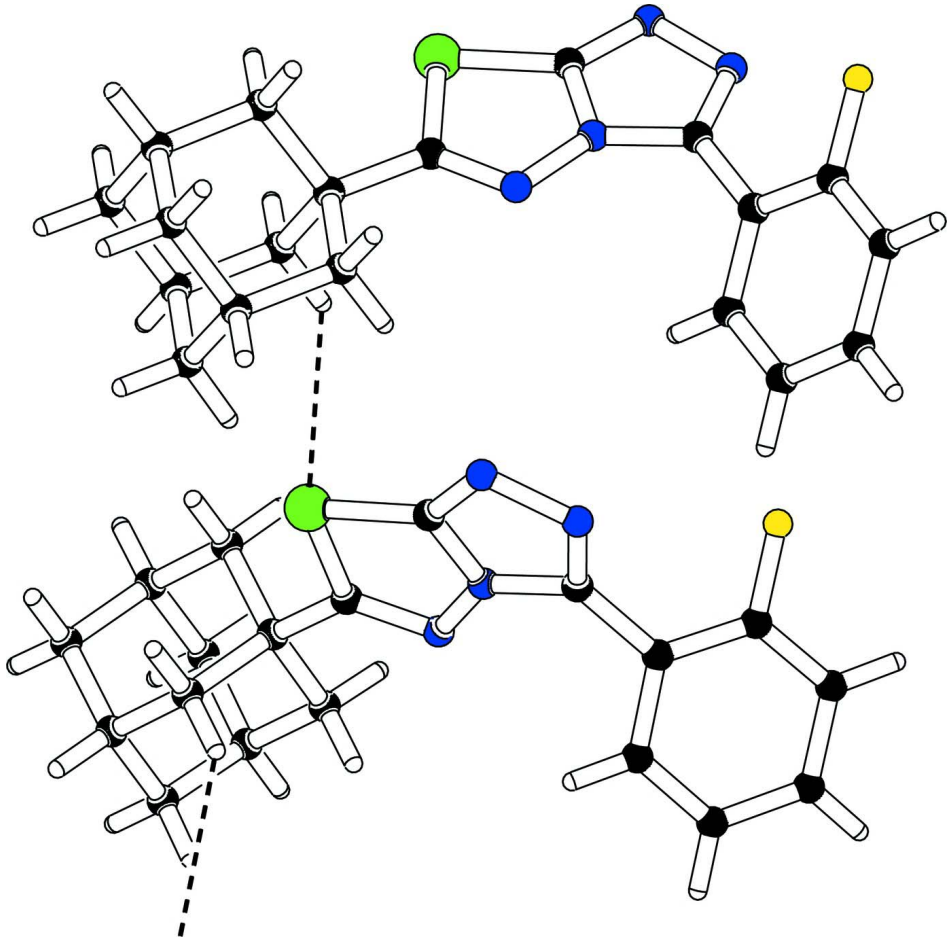

Figure 2

Partial packing diagram for (I) showing the C—H···S interaction as a dashed line.

6-(1-Adamantyl)-3-(2-fluorophenyl)-1,2,4- triazolo[3,4-*b*][1,3,4]thiadiazole

Crystal data

$C_{19}H_{19}FN_4S$
$M_r = 354.44$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.2684\ (9)$ Å
$b = 12.4293\ (9)$ Å
$c = 20.2231\ (15)$ Å
$V = 3335.1\ (4)$ Å^3
$Z = 8$
$F(000) = 1488$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3116 reflections
$\theta = 2.5–29.1°$
$\mu = 0.21$ mm^{-1}
$T = 296$ K
Prism, colourless
0.25 × 0.22 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.40 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.945$, $T_{max} = 0.956$
22695 measured reflections
4486 independent reflections
3116 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$

θ_{max} = 29.1°, θ_{min} = 2.5°
h = −12→18
k = −17→14
l = −26→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.136
S = 1.04
4486 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 1.3259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.25232 (4)	−0.15058 (4)	0.23126 (2)	0.0517 (2)
F1	0.35571 (14)	−0.27396 (11)	0.52074 (7)	0.0839 (6)
N1	0.20243 (13)	−0.22822 (13)	0.41446 (9)	0.0543 (6)
N2	0.17459 (14)	−0.24778 (14)	0.34844 (9)	0.0591 (6)
N3	0.29443 (10)	−0.12526 (11)	0.35182 (7)	0.0360 (4)
N4	0.36117 (10)	−0.05549 (11)	0.32199 (7)	0.0343 (4)
C1	0.32252 (13)	−0.10525 (14)	0.47314 (9)	0.0392 (5)
C2	0.36251 (16)	−0.16551 (17)	0.52410 (10)	0.0517 (6)
C3	0.41073 (19)	−0.1200 (2)	0.57717 (10)	0.0639 (8)
C4	0.41784 (17)	−0.0094 (2)	0.58048 (10)	0.0611 (8)
C5	0.37749 (16)	0.05301 (18)	0.53119 (10)	0.0549 (7)
C6	0.33120 (14)	0.00584 (15)	0.47758 (9)	0.0463 (6)
C7	0.27374 (13)	−0.15494 (14)	0.41576 (9)	0.0403 (5)
C8	0.23167 (13)	−0.18403 (14)	0.31343 (10)	0.0437 (5)
C9	0.34740 (12)	−0.06062 (13)	0.25887 (8)	0.0348 (5)
C10	0.40431 (12)	0.00535 (13)	0.20943 (8)	0.0337 (4)
C11	0.48759 (15)	0.07039 (18)	0.24376 (9)	0.0504 (6)
C12	0.54359 (15)	0.13979 (18)	0.19241 (10)	0.0543 (7)
C13	0.47109 (16)	0.21626 (17)	0.15982 (11)	0.0581 (7)
C14	0.38813 (17)	0.15387 (18)	0.12638 (12)	0.0626 (8)
C15	0.33138 (15)	0.08502 (16)	0.17677 (11)	0.0527 (6)
C16	0.4512 (2)	−0.06639 (17)	0.15637 (11)	0.0657 (8)
C17	0.5082 (3)	0.0039 (2)	0.10590 (12)	0.0802 (9)
C18	0.59042 (18)	0.0674 (2)	0.14102 (13)	0.0730 (9)

C19	0.4329 (3)	0.0822 (2)	0.07399 (11)	0.0855 (10)
H3	0.43812	−0.16293	0.61028	0.0767*
H4	0.45004	0.02286	0.61619	0.0733*
H5	0.38143	0.12757	0.53400	0.0658*
H6	0.30545	0.04888	0.44397	0.0555*
H11A	0.45818	0.11629	0.27742	0.0604*
H11B	0.53468	0.02185	0.26512	0.0604*
H12	0.59673	0.18097	0.21460	0.0651*
H13A	0.44245	0.26409	0.19273	0.0697*
H13B	0.50652	0.25966	0.12744	0.0697*
H14	0.34099	0.20433	0.10564	0.0751*
H15A	0.30145	0.13091	0.21022	0.0633*
H15B	0.27764	0.04595	0.15483	0.0633*
H16A	0.49735	−0.11705	0.17670	0.0789*
H16B	0.39877	−0.10692	0.13405	0.0789*
H17	0.53836	−0.04191	0.07176	0.0963*
H18A	0.62742	0.11032	0.10915	0.0876*
H18B	0.63734	0.01826	0.16203	0.0876*
H19A	0.37972	0.04208	0.05216	0.1027*
H19B	0.46694	0.12570	0.04103	0.1027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0578 (3)	0.0481 (3)	0.0492 (3)	−0.0163 (2)	−0.0141 (2)	−0.0060 (2)
F1	0.1293 (14)	0.0492 (8)	0.0733 (9)	0.0040 (8)	−0.0198 (9)	0.0189 (7)
N1	0.0552 (10)	0.0455 (9)	0.0623 (11)	−0.0141 (8)	−0.0018 (8)	0.0070 (8)
N2	0.0611 (10)	0.0483 (9)	0.0678 (12)	−0.0202 (8)	−0.0068 (9)	0.0020 (9)
N3	0.0342 (7)	0.0312 (7)	0.0427 (8)	−0.0025 (5)	−0.0031 (6)	−0.0002 (6)
N4	0.0330 (7)	0.0324 (7)	0.0375 (7)	−0.0016 (5)	−0.0019 (6)	−0.0014 (6)
C1	0.0351 (8)	0.0425 (9)	0.0401 (9)	−0.0011 (7)	0.0052 (7)	0.0042 (7)
C2	0.0615 (12)	0.0487 (11)	0.0450 (10)	0.0004 (9)	0.0043 (9)	0.0110 (9)
C3	0.0733 (15)	0.0777 (16)	0.0407 (10)	0.0016 (12)	−0.0069 (10)	0.0148 (10)
C4	0.0616 (13)	0.0810 (16)	0.0406 (10)	−0.0128 (12)	0.0007 (9)	−0.0047 (10)
C5	0.0585 (12)	0.0528 (12)	0.0533 (12)	−0.0067 (10)	0.0026 (10)	−0.0077 (9)
C6	0.0470 (10)	0.0432 (10)	0.0487 (10)	−0.0015 (8)	−0.0022 (8)	0.0024 (8)
C7	0.0390 (9)	0.0342 (8)	0.0478 (10)	−0.0005 (7)	0.0006 (7)	0.0048 (7)
C8	0.0425 (9)	0.0356 (9)	0.0530 (10)	−0.0064 (7)	−0.0083 (8)	−0.0036 (8)
C9	0.0338 (8)	0.0313 (7)	0.0394 (9)	0.0013 (6)	−0.0055 (7)	−0.0054 (7)
C10	0.0355 (8)	0.0340 (8)	0.0315 (7)	0.0043 (6)	−0.0038 (6)	−0.0048 (6)
C11	0.0423 (10)	0.0682 (13)	0.0406 (9)	−0.0147 (9)	−0.0045 (8)	0.0014 (9)
C12	0.0401 (10)	0.0728 (14)	0.0499 (11)	−0.0137 (9)	−0.0001 (8)	0.0052 (10)
C13	0.0550 (12)	0.0478 (11)	0.0716 (14)	−0.0041 (9)	0.0134 (11)	0.0044 (10)
C14	0.0527 (12)	0.0602 (13)	0.0748 (15)	0.0024 (10)	−0.0127 (11)	0.0291 (12)
C15	0.0402 (10)	0.0453 (10)	0.0727 (13)	0.0009 (8)	−0.0095 (9)	0.0140 (10)
C16	0.0922 (18)	0.0451 (11)	0.0599 (13)	0.0105 (11)	0.0243 (12)	−0.0122 (10)
C17	0.123 (2)	0.0619 (15)	0.0558 (13)	0.0071 (15)	0.0433 (15)	−0.0135 (12)
C18	0.0537 (13)	0.0819 (17)	0.0834 (17)	0.0217 (12)	0.0285 (12)	0.0241 (14)

C19	0.114 (2)	0.105 (2)	0.0374 (11)	−0.0375 (19)	−0.0114 (13)	0.0115 (13)

Geometric parameters (Å, º)

S1—C8	1.735 (2)	C14—C15	1.529 (3)
S1—C9	1.7758 (17)	C14—C19	1.506 (4)
F1—C2	1.353 (3)	C16—C17	1.542 (4)
N1—N2	1.407 (3)	C17—C18	1.522 (4)
N1—C7	1.314 (2)	C17—C19	1.537 (5)
N2—C8	1.305 (3)	C3—H3	0.9300
N3—N4	1.3784 (19)	C4—H4	0.9300
N3—C7	1.372 (2)	C5—H5	0.9300
N3—C8	1.353 (2)	C6—H6	0.9300
N4—C9	1.291 (2)	C11—H11A	0.9700
C1—C2	1.380 (3)	C11—H11B	0.9700
C1—C6	1.389 (3)	C12—H12	0.9800
C1—C7	1.465 (3)	C13—H13A	0.9700
C2—C3	1.372 (3)	C13—H13B	0.9700
C3—C4	1.380 (4)	C14—H14	0.9800
C4—C5	1.372 (3)	C15—H15A	0.9700
C5—C6	1.377 (3)	C15—H15B	0.9700
C9—C10	1.497 (2)	C16—H16A	0.9700
C10—C11	1.535 (3)	C16—H16B	0.9700
C10—C15	1.534 (3)	C17—H17	0.9800
C10—C16	1.528 (3)	C18—H18A	0.9700
C11—C12	1.541 (3)	C18—H18B	0.9700
C12—C13	1.504 (3)	C19—H19A	0.9700
C12—C18	1.509 (3)	C19—H19B	0.9700
C13—C14	1.507 (3)		
C8—S1—C9	87.82 (8)	C2—C3—H3	121.00
N2—N1—C7	109.15 (16)	C4—C3—H3	121.00
N1—N2—C8	104.93 (16)	C3—C4—H4	120.00
N4—N3—C7	135.23 (14)	C5—C4—H4	120.00
N4—N3—C8	118.95 (14)	C4—C5—H5	120.00
C7—N3—C8	105.81 (14)	C6—C5—H5	120.00
N3—N4—C9	108.10 (13)	C1—C6—H6	120.00
C2—C1—C6	117.36 (17)	C5—C6—H6	120.00
C2—C1—C7	122.17 (17)	C10—C11—H11A	110.00
C6—C1—C7	120.47 (16)	C10—C11—H11B	110.00
F1—C2—C1	118.53 (18)	C12—C11—H11A	110.00
F1—C2—C3	118.78 (19)	C12—C11—H11B	110.00
C1—C2—C3	122.7 (2)	H11A—C11—H11B	108.00
C2—C3—C4	118.7 (2)	C11—C12—H12	109.00
C3—C4—C5	120.1 (2)	C13—C12—H12	109.00
C4—C5—C6	120.4 (2)	C18—C12—H12	109.00
C1—C6—C5	120.75 (18)	C12—C13—H13A	110.00
N1—C7—N3	108.16 (16)	C12—C13—H13B	110.00

N1—C7—C1	128.78 (17)	C14—C13—H13A	110.00
N3—C7—C1	122.99 (15)	C14—C13—H13B	110.00
S1—C8—N2	139.20 (16)	H13A—C13—H13B	108.00
S1—C8—N3	108.85 (13)	C13—C14—H14	109.00
N2—C8—N3	111.95 (18)	C15—C14—H14	109.00
S1—C9—N4	116.26 (12)	C19—C14—H14	109.00
S1—C9—C10	119.54 (12)	C10—C15—H15A	110.00
N4—C9—C10	124.18 (15)	C10—C15—H15B	110.00
C9—C10—C11	110.45 (14)	C14—C15—H15A	110.00
C9—C10—C15	108.84 (14)	C14—C15—H15B	110.00
C9—C10—C16	110.78 (14)	H15A—C15—H15B	108.00
C11—C10—C15	107.99 (15)	C10—C16—H16A	110.00
C11—C10—C16	109.38 (16)	C10—C16—H16B	110.00
C15—C10—C16	109.35 (15)	C17—C16—H16A	110.00
C10—C11—C12	109.70 (15)	C17—C16—H16B	110.00
C11—C12—C13	109.91 (17)	H16A—C16—H16B	108.00
C11—C12—C18	109.21 (18)	C16—C17—H17	110.00
C13—C12—C18	109.78 (18)	C18—C17—H17	110.00
C12—C13—C14	109.79 (18)	C19—C17—H17	110.00
C13—C14—C15	110.41 (19)	C12—C18—H18A	110.00
C13—C14—C19	109.4 (2)	C12—C18—H18B	110.00
C15—C14—C19	109.39 (19)	C17—C18—H18A	110.00
C10—C15—C14	109.73 (16)	C17—C18—H18B	110.00
C10—C16—C17	109.51 (17)	H18A—C18—H18B	108.00
C16—C17—C18	109.7 (2)	C14—C19—H19A	110.00
C16—C17—C19	108.5 (3)	C14—C19—H19B	110.00
C18—C17—C19	109.5 (2)	C17—C19—H19A	110.00
C12—C18—C17	109.6 (2)	C17—C19—H19B	110.00
C14—C19—C17	109.61 (19)	H19A—C19—H19B	108.00

C9—S1—C8—N2	−179.0 (2)	C4—C5—C6—C1	1.5 (3)
C9—S1—C8—N3	1.05 (13)	S1—C9—C10—C11	−175.71 (12)
C8—S1—C9—N4	−0.64 (14)	S1—C9—C10—C15	65.90 (17)
C8—S1—C9—C10	−179.31 (14)	S1—C9—C10—C16	−54.36 (19)
C7—N1—N2—C8	−0.1 (2)	N4—C9—C10—C11	5.7 (2)
N2—N1—C7—N3	−0.2 (2)	N4—C9—C10—C15	−112.66 (18)
N2—N1—C7—C1	176.70 (17)	N4—C9—C10—C16	127.08 (18)
N1—N2—C8—S1	−179.67 (17)	C9—C10—C11—C12	−178.63 (15)
N1—N2—C8—N3	0.3 (2)	C15—C10—C11—C12	−59.7 (2)
C7—N3—N4—C9	179.60 (18)	C16—C10—C11—C12	59.2 (2)
C8—N3—N4—C9	0.9 (2)	C9—C10—C15—C14	179.60 (16)
N4—N3—C7—N1	−178.48 (16)	C11—C10—C15—C14	59.7 (2)
N4—N3—C7—C1	4.4 (3)	C16—C10—C15—C14	−59.3 (2)
C8—N3—C7—N1	0.33 (19)	C9—C10—C16—C17	179.4 (2)
C8—N3—C7—C1	−176.77 (16)	C11—C10—C16—C17	−58.6 (2)
N4—N3—C8—S1	−1.38 (18)	C15—C10—C16—C17	59.5 (2)
N4—N3—C8—N2	178.67 (15)	C10—C11—C12—C13	60.2 (2)
C7—N3—C8—S1	179.58 (12)	C10—C11—C12—C18	−60.3 (2)

C7—N3—C8—N2	−0.4 (2)	C11—C12—C13—C14	−59.2 (2)
N3—N4—C9—S1	0.02 (17)	C18—C12—C13—C14	61.0 (2)
N3—N4—C9—C10	178.62 (14)	C11—C12—C18—C17	61.0 (2)
C6—C1—C2—F1	−179.52 (18)	C13—C12—C18—C17	−59.6 (2)
C6—C1—C2—C3	−1.0 (3)	C12—C13—C14—C15	59.4 (2)
C7—C1—C2—F1	−0.3 (3)	C12—C13—C14—C19	−61.0 (2)
C7—C1—C2—C3	178.2 (2)	C13—C14—C15—C10	−60.1 (2)
C2—C1—C6—C5	−0.4 (3)	C19—C14—C15—C10	60.3 (2)
C7—C1—C6—C5	−179.61 (18)	C13—C14—C19—C17	59.7 (3)
C2—C1—C7—N1	50.7 (3)	C15—C14—C19—C17	−61.4 (3)
C2—C1—C7—N3	−132.83 (19)	C10—C16—C17—C18	59.5 (3)
C6—C1—C7—N1	−130.1 (2)	C10—C16—C17—C19	−60.1 (2)
C6—C1—C7—N3	46.3 (3)	C16—C17—C18—C12	−60.8 (3)
F1—C2—C3—C4	179.9 (2)	C19—C17—C18—C12	58.2 (3)
C1—C2—C3—C4	1.3 (3)	C16—C17—C19—C14	61.2 (3)
C2—C3—C4—C5	−0.3 (3)	C18—C17—C19—C14	−58.5 (3)
C3—C4—C5—C6	−1.1 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···S1^{i}	0.97	2.84	3.640 (2)	140
C12—H12···*Cg*1^{ii}	0.98	2.90	3.713 (2)	140
C18—H18*B*···*Cg*1^{iii}	0.97	2.83	3.787 (3)	170

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