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5-(4-Chlorophenyl)-3-(2,4-dimethylthiazol-5-yl)-1,2,4-triazolo[3,4-*a*]isoquinoline

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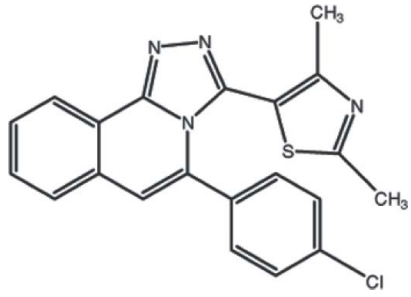
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.111; data-to-parameter ratio = 14.0.

In the title molecule, $C_{21}H_{15}ClN_4S$, the triazoloisoquinoline ring system is approximately planar, with an r.m.s. deviation of 0.054 (2) Å and a maximum deviation of 0.098 (2) Å from the mean plane for the triazole ring C atom that is bonded to the thiazole ring. The thiazole and benzene rings are twisted by 66.36 (7) and 56.32 (7)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. In the crystal structure, molecules are linked by intermolecular C—H···N interactions along the *a* axis. The molecular conformation is stabilized by a weak intramolecular π–π interaction involving the thiazole and benzene rings, with a centroid–centroid distance of 3.6546 (11) Å. In addition, two other intermolecular π–π stacking interactions are observed, between the triazole and benzene rings and between the dihydropyridine and benzene rings [centroid–centroid distances = 3.6489 (11) and 3.5967 (10) Å, respectively].

Related literature

For the synthesis and antihelmintic activity of triazolo compounds similar to the title compound, see: Nadkarni *et al.* (2001). For related structures, see: Hui *et al.* (1999); Khan *et al.* (2010); Zou *et al.* (2004).



Experimental

Crystal data

$C_{21}H_{15}ClN_4S$
M_r = 390.89
Triclinic, $P\overline{1}$
a = 7.8286 (5) Å
b = 8.1754 (6) Å
c = 15.1264 (9) Å
α = 93.514 (5)°
β = 94.805 (5)°
γ = 105.963 (6)°
V = 923.92 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 290 K
0.40 × 0.25 × 0.24 mm

Data collection

Oxford Xcalibur diffractometer with an Eos (Nova) CCD detector
Absorption correction: multi-scan (*CrysAlis PRO RED*; Oxford Diffraction, 2009)
T_{min} = 0.851, T_{max} = 0.924
19579 measured reflections
3439 independent reflections
2518 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.111
S = 1.09
3439 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···N2^{i}	0.93	2.62	3.495 (2)	158
C8—H8···N3^{i}	0.93	2.51	3.383 (2)	156

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the FIST program for data collection on the single-crystal diffractometer at SSCU, IISc, Bangalore. We also thank Professor T. N. Guru Row, IISc, Bangalore, for his help with the data collection. FNK thanks the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2293).

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supporting information

Acta Cryst. (2010). E**66**, o1056–o1057 [https://doi.org/10.1107/S160053681001278X]

5-(4-Chlorophenyl)-3-(2,4-dimethylthiazol-5-yl)-1,2,4-triazolo[3,4-*a*]isoquinoline

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S1. Comment

Drugs including alprazolam (tranquilizer), estazolam (hypnotic, sedative, tranquilizer), rilmazafon (hypnotic, anxiolytic, used in the case of neurotic insomnia), benatradin (diuretic), trapidil (hypotensive), trazodon (antidepressant, anxiolytic), etoperidone (antidepressant), nefazodone (antidepressant, 5-HT2 A-antagonist), anastazole (antineoplastic, non-steroidal aromatase inhibitor), letrozole (antineoplastic, aromatase inhibitor), ribavirin (antiviral), fluconazole, itraconazole, terconazole (antifungal) possess 1,2,4-Triazole as the structural element. Besides, it follows from the literature data that 1,2,4-triazoles and their fused systems show antibacterial, antifungal and antiflammatory properties. As part of our search for new isoquinoline analogues, we focused on synthesis of titled compounds and the crystal structure is reported.

In the title molecule (I), Fig. 1, the triazoloisoquinoline ring system (N1–N3/C1–C9/C16) is nearly planar, with an r.m.s. deviation of 0.054 (2) Å and a maximum deviation of 0.098 (2) Å from the mean plane for the triazole ring C16 atom which is bonded to the thiazole ring (S1/N4/C17/C18/C20). The thiazole (S1/N4/C17/C18/C20) and benzene (C10—C15) rings are twisted by 66.36 (7) and 56.32 (7)°, respectively, with respect to the mean plane of the triazoloisoquinoline ring system. The thiazole ring forms a dihedral angle of 23.34 (9)° with benzene ring.

In the crystal structure of (I), molecules are linked by intermolecular C—H···N interactions along the [100] direction (Table 1, Fig. 2). Furthermore, π-π interactions [Cg1···Cg5(x, y, z) = 3.6546 (11) Å and Cg2···Cg4(2-x, 2-y, 1-z) = 3.6489 (11) Å. Where Cg1, Cg2, Cg4 and Cg5 are the centroids of the S1/N4/C17/C18/C20, N1–N3/C1/C16, C2–C7 and C10–C15 rings, respectively] are observed.

S2. Experimental

2-(3-(4-Chlorophenylisoquinolin-1-yl)hydrazine (1 mmol) was condensed with 2,4-dimethylthiazole-5-carbaldehyde (1.1 mmol) under refluxing conditions in isopropanol (10 ml) solvent to give the corresponding hydrazone in high yield. After removal of the solvent the compound was then oxidatively cyclized in nitrobenzene (10 ml) at 473 K. The product was recrystallized from dichlomethane to give block-shaped crystals.

S3. Refinement

All H atoms were placed in calculated positions with C–H = 0.93 and 0.96 Å and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2 or 1.5U_{eq}(C).

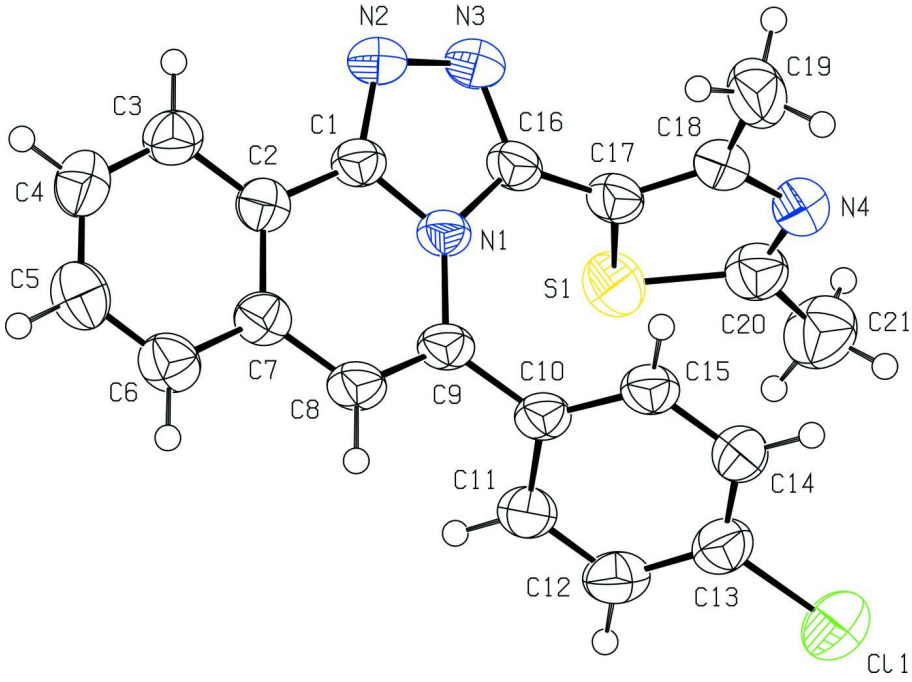

Figure 1

The title molecule with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

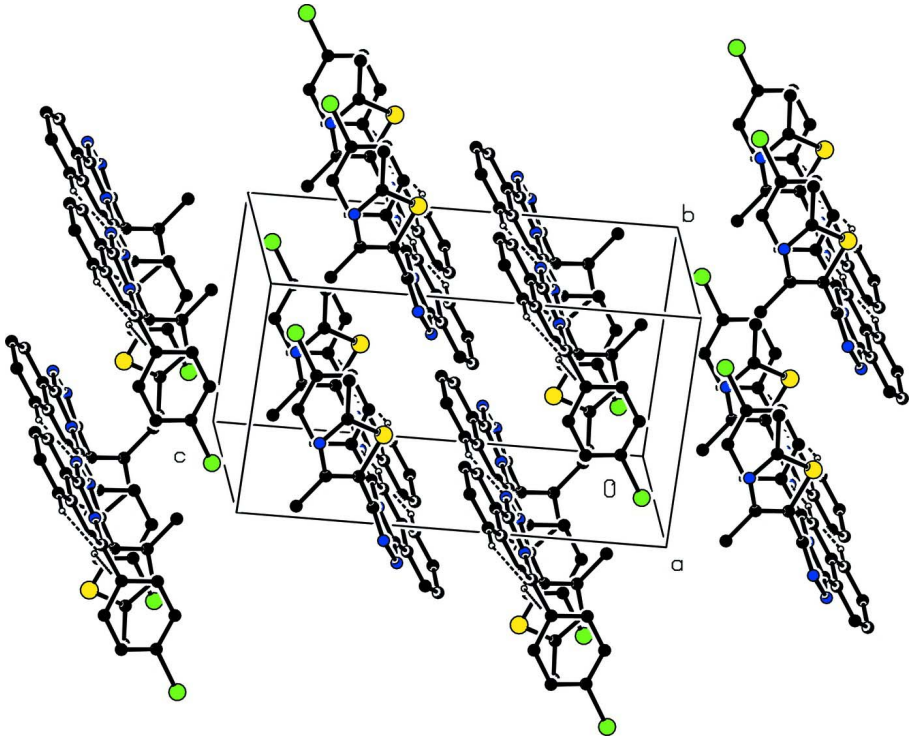

Figure 2

View of the packing diagram and the hydrogen bonding of (I) down the [100] direction. H atoms not involved in the motif shown have been omitted for clarity.

5-(4-Chlorophenyl)-3-(2,4-dimethylthiazol-5-yl)-1,2,4- triazolo[3,4-*a*]isoquinoline

Crystal data

$C_{21}H_{15}ClN_4S$
$M_r = 390.89$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.8286$ (5) Å
$b = 8.1754$ (6) Å
$c = 15.1264$ (9) Å
$\alpha = 93.514$ (5)°
$\beta = 94.805$ (5)°
$\gamma = 105.963$ (6)°
$V = 923.92$ (11) Å^3
$Z = 2$
$F(000) = 404$
$D_x = 1.405$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 954 reflections
$\theta = 2.0$–$20.4°$
$\mu = 0.33$ mm^{-1}
$T = 290$ K
Block, pale yellow
0.40 × 0.25 × 0.24 mm

Data collection

Oxford Xcalibur Eos (Nova) CCD detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)
$T_{min} = 0.851$, $T_{max} = 0.924$
19579 measured reflections
3439 independent reflections
2518 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.0°$
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.111$
$S = 1.09$
3439 reflections
246 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
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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. 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	0.55766 (7)	0.44377 (7)	0.27355 (3)	0.05951 (19)
Cl1	0.90834 (9)	0.16939 (8)	0.06573 (5)	0.0843 (2)
N1	0.84486 (17)	0.86756 (18)	0.31082 (9)	0.0404 (3)

N2	0.69901 (19)	1.0456 (2)	0.36035 (10)	0.0527 (4)
N3	0.57837 (19)	0.9079 (2)	0.31201 (11)	0.0552 (4)
N4	0.4093 (2)	0.4452 (2)	0.11718 (11)	0.0566 (4)
C1	0.8562 (2)	1.0182 (2)	0.36077 (11)	0.0422 (4)
C2	1.0238 (2)	1.1181 (2)	0.40777 (11)	0.0424 (4)
C3	1.0384 (3)	1.2657 (2)	0.46264 (12)	0.0518 (5)
H3	0.9390	1.3053	0.4684	0.062*
C4	1.2006 (3)	1.3523 (2)	0.50822 (13)	0.0567 (5)
H4	1.2103	1.4503	0.5452	0.068*
C5	1.3493 (3)	1.2952 (3)	0.49973 (13)	0.0572 (5)
H5	1.4581	1.3545	0.5313	0.069*
C6	1.3375 (2)	1.1514 (3)	0.44506 (13)	0.0542 (5)
H6	1.4388	1.1150	0.4390	0.065*
C7	1.1733 (2)	1.0589 (2)	0.39819 (11)	0.0444 (4)
C8	1.1543 (2)	0.9065 (2)	0.34138 (12)	0.0466 (4)
H8	1.2558	0.8710	0.3341	0.056*
C9	0.9971 (2)	0.8117 (2)	0.29783 (11)	0.0423 (4)
C10	0.9794 (2)	0.6564 (2)	0.23864 (11)	0.0428 (4)
C11	1.0353 (2)	0.5235 (3)	0.27137 (13)	0.0519 (5)
H11	1.0870	0.5347	0.3299	0.062*
C12	1.0157 (3)	0.3744 (3)	0.21852 (14)	0.0573 (5)
H12	1.0532	0.2853	0.2412	0.069*
C13	0.9398 (3)	0.3592 (3)	0.13168 (13)	0.0541 (5)
C14	0.8902 (2)	0.4919 (3)	0.09643 (12)	0.0527 (5)
H14	0.8433	0.4820	0.0371	0.063*
C15	0.9105 (2)	0.6405 (2)	0.14989 (12)	0.0475 (4)
H15	0.8776	0.7311	0.1262	0.057*
C16	0.6634 (2)	0.8009 (2)	0.28300 (11)	0.0453 (4)
C17	0.5732 (2)	0.6376 (2)	0.23238 (12)	0.0471 (4)
C18	0.4858 (2)	0.6136 (2)	0.14858 (12)	0.0498 (5)
C19	0.4738 (3)	0.7494 (3)	0.09026 (15)	0.0764 (7)
H19A	0.3563	0.7645	0.0884	0.115*
H19B	0.4969	0.7176	0.0312	0.115*
H19C	0.5605	0.8544	0.1132	0.115*
C20	0.4383 (2)	0.3425 (3)	0.17513 (14)	0.0558 (5)
C21	0.3769 (4)	0.1526 (3)	0.16023 (18)	0.0799 (7)
H21A	0.2505	0.1137	0.1641	0.120*
H21B	0.4382	0.1043	0.2048	0.120*
H21C	0.4023	0.1173	0.1023	0.120*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0593 (3)	0.0633 (4)	0.0552 (3)	0.0153 (3)	0.0034 (2)	0.0122 (2)
Cl1	0.0961 (5)	0.0658 (4)	0.0907 (5)	0.0316 (3)	−0.0026 (3)	−0.0189 (3)
N1	0.0364 (8)	0.0490 (9)	0.0405 (8)	0.0185 (7)	0.0070 (6)	0.0052 (6)
N2	0.0451 (9)	0.0614 (10)	0.0577 (10)	0.0276 (8)	0.0029 (7)	−0.0021 (8)
N3	0.0402 (9)	0.0680 (11)	0.0614 (10)	0.0249 (8)	0.0008 (7)	−0.0027 (8)

N4	0.0550 (10)	0.0589 (11)	0.0559 (10)	0.0203 (9)	−0.0029 (8)	−0.0027 (8)
C1	0.0411 (10)	0.0502 (10)	0.0406 (9)	0.0200 (8)	0.0084 (7)	0.0062 (8)
C2	0.0439 (10)	0.0467 (10)	0.0384 (9)	0.0135 (8)	0.0085 (7)	0.0095 (8)
C3	0.0581 (12)	0.0523 (11)	0.0503 (11)	0.0232 (10)	0.0079 (9)	0.0074 (9)
C4	0.0691 (13)	0.0485 (11)	0.0486 (11)	0.0115 (10)	0.0044 (9)	0.0009 (9)
C5	0.0509 (12)	0.0561 (13)	0.0566 (12)	0.0024 (10)	0.0006 (9)	0.0088 (10)
C6	0.0384 (10)	0.0640 (13)	0.0588 (12)	0.0106 (9)	0.0084 (8)	0.0072 (10)
C7	0.0399 (10)	0.0520 (11)	0.0435 (10)	0.0135 (8)	0.0111 (7)	0.0098 (8)
C8	0.0342 (9)	0.0601 (12)	0.0501 (10)	0.0192 (9)	0.0110 (8)	0.0049 (9)
C9	0.0364 (9)	0.0548 (11)	0.0422 (9)	0.0209 (8)	0.0116 (7)	0.0083 (8)
C10	0.0362 (9)	0.0540 (11)	0.0435 (10)	0.0190 (8)	0.0112 (7)	0.0054 (8)
C11	0.0526 (11)	0.0644 (13)	0.0468 (11)	0.0290 (10)	0.0064 (8)	0.0078 (9)
C12	0.0618 (12)	0.0573 (12)	0.0628 (13)	0.0308 (11)	0.0119 (10)	0.0114 (10)
C13	0.0511 (11)	0.0549 (12)	0.0586 (12)	0.0183 (10)	0.0109 (9)	−0.0014 (9)
C14	0.0518 (11)	0.0665 (13)	0.0436 (10)	0.0232 (10)	0.0066 (8)	0.0011 (9)
C15	0.0457 (10)	0.0586 (12)	0.0454 (10)	0.0242 (9)	0.0099 (8)	0.0085 (9)
C16	0.0344 (9)	0.0608 (12)	0.0442 (10)	0.0189 (9)	0.0041 (7)	0.0053 (9)
C17	0.0354 (9)	0.0592 (12)	0.0495 (11)	0.0181 (9)	0.0048 (8)	0.0037 (9)
C18	0.0460 (10)	0.0538 (11)	0.0521 (11)	0.0215 (9)	−0.0021 (8)	−0.0002 (9)
C19	0.0994 (17)	0.0625 (14)	0.0660 (14)	0.0318 (13)	−0.0244 (12)	0.0001 (11)
C20	0.0501 (11)	0.0564 (12)	0.0623 (13)	0.0169 (10)	0.0088 (9)	0.0039 (10)
C21	0.0942 (18)	0.0585 (14)	0.0864 (17)	0.0212 (13)	0.0081 (13)	0.0040 (12)

Geometric parameters (Å, º)

S1—C17	1.7150 (19)	C8—C9	1.351 (2)
S1—C20	1.722 (2)	C8—H8	0.9300
Cl1—C13	1.7387 (19)	C9—C10	1.475 (2)
N1—C1	1.382 (2)	C10—C11	1.382 (2)
N1—C16	1.392 (2)	C10—C15	1.389 (2)
N1—C9	1.413 (2)	C11—C12	1.381 (3)
N2—C1	1.310 (2)	C11—H11	0.9300
N2—N3	1.376 (2)	C12—C13	1.379 (3)
N3—C16	1.313 (2)	C12—H12	0.9300
N4—C20	1.299 (3)	C13—C14	1.371 (3)
N4—C18	1.378 (2)	C14—C15	1.381 (2)
C1—C2	1.441 (2)	C14—H14	0.9300
C2—C3	1.394 (2)	C15—H15	0.9300
C2—C7	1.399 (2)	C16—C17	1.460 (2)
C3—C4	1.374 (3)	C17—C18	1.365 (3)
C3—H3	0.9300	C18—C19	1.477 (3)
C4—C5	1.380 (3)	C19—H19A	0.9600
C4—H4	0.9300	C19—H19B	0.9600
C5—C6	1.372 (2)	C19—H19C	0.9600
C5—H5	0.9300	C20—C21	1.490 (3)
C6—C7	1.405 (3)	C21—H21A	0.9600
C6—H6	0.9300	C21—H21B	0.9600
C7—C8	1.435 (2)	C21—H21C	0.9600

C17—S1—C20	89.71 (9)	C12—C11—H11	119.5
C1—N1—C16	104.18 (13)	C10—C11—H11	119.5
C1—N1—C9	122.02 (14)	C13—C12—C11	119.11 (18)
C16—N1—C9	133.80 (15)	C13—C12—H12	120.4
C1—N2—N3	106.96 (14)	C11—C12—H12	120.4
C16—N3—N2	109.14 (14)	C14—C13—C12	121.03 (18)
C20—N4—C18	111.44 (17)	C14—C13—Cl1	119.56 (16)
N2—C1—N1	110.74 (15)	C12—C13—Cl1	119.41 (16)
N2—C1—C2	128.52 (16)	C13—C14—C15	119.30 (18)
N1—C1—C2	120.68 (14)	C13—C14—H14	120.3
C3—C2—C7	120.43 (17)	C15—C14—H14	120.3
C3—C2—C1	122.28 (16)	C14—C15—C10	120.84 (18)
C7—C2—C1	117.26 (16)	C14—C15—H15	119.6
C4—C3—C2	119.62 (18)	C10—C15—H15	119.6
C4—C3—H3	120.2	N3—C16—N1	108.91 (16)
C2—C3—H3	120.2	N3—C16—C17	123.14 (15)
C3—C4—C5	120.64 (19)	N1—C16—C17	127.92 (15)
C3—C4—H4	119.7	C18—C17—C16	126.79 (17)
C5—C4—H4	119.7	C18—C17—S1	109.80 (14)
C6—C5—C4	120.41 (19)	C16—C17—S1	123.38 (14)
C6—C5—H5	119.8	C17—C18—N4	114.72 (17)
C4—C5—H5	119.8	C17—C18—C19	125.94 (18)
C5—C6—C7	120.40 (18)	N4—C18—C19	119.29 (17)
C5—C6—H6	119.8	C18—C19—H19A	109.5
C7—C6—H6	119.8	C18—C19—H19B	109.5
C2—C7—C6	118.48 (17)	H19A—C19—H19B	109.5
C2—C7—C8	119.24 (16)	C18—C19—H19C	109.5
C6—C7—C8	122.28 (16)	H19A—C19—H19C	109.5
C9—C8—C7	123.62 (16)	H19B—C19—H19C	109.5
C9—C8—H8	118.2	N4—C20—C21	124.4 (2)
C7—C8—H8	118.2	N4—C20—S1	114.31 (16)
C8—C9—N1	116.99 (16)	C21—C20—S1	121.26 (17)
C8—C9—C10	123.21 (15)	C20—C21—H21A	109.5
N1—C9—C10	119.80 (14)	C20—C21—H21B	109.5
C11—C10—C15	118.60 (17)	H21A—C21—H21B	109.5
C11—C10—C9	119.53 (16)	C20—C21—H21C	109.5
C15—C10—C9	121.87 (16)	H21A—C21—H21C	109.5
C12—C11—C10	121.00 (18)	H21B—C21—H21C	109.5

C1—N2—N3—C16	−0.8 (2)	N1—C9—C10—C15	57.7 (2)
N3—N2—C1—N1	2.2 (2)	C15—C10—C11—C12	−3.1 (3)
N3—N2—C1—C2	−174.89 (17)	C9—C10—C11—C12	178.05 (16)
C16—N1—C1—N2	−2.68 (19)	C10—C11—C12—C13	0.3 (3)
C9—N1—C1—N2	177.60 (14)	C11—C12—C13—C14	2.5 (3)
C16—N1—C1—C2	174.71 (15)	C11—C12—C13—Cl1	−178.02 (15)
C9—N1—C1—C2	−5.0 (2)	C12—C13—C14—C15	−2.5 (3)
N2—C1—C2—C3	0.4 (3)	Cl1—C13—C14—C15	178.05 (13)

N1—C1—C2—C3	−176.44 (16)	C13—C14—C15—C10	−0.4 (3)
N2—C1—C2—C7	178.86 (17)	C11—C10—C15—C14	3.1 (3)
N1—C1—C2—C7	2.0 (2)	C9—C10—C15—C14	−178.05 (15)
C7—C2—C3—C4	−0.7 (3)	N2—N3—C16—N1	−0.8 (2)
C1—C2—C3—C4	177.71 (16)	N2—N3—C16—C17	177.39 (16)
C2—C3—C4—C5	0.4 (3)	C1—N1—C16—N3	2.09 (18)
C3—C4—C5—C6	0.4 (3)	C9—N1—C16—N3	−178.24 (17)
C4—C5—C6—C7	−1.1 (3)	C1—N1—C16—C17	−176.03 (17)
C3—C2—C7—C6	0.1 (3)	C9—N1—C16—C17	3.6 (3)
C1—C2—C7—C6	−178.40 (15)	N3—C16—C17—C18	66.9 (3)
C3—C2—C7—C8	179.91 (16)	N1—C16—C17—C18	−115.2 (2)
C1—C2—C7—C8	1.4 (2)	N3—C16—C17—S1	−111.10 (18)
C5—C6—C7—C2	0.8 (3)	N1—C16—C17—S1	66.8 (2)
C5—C6—C7—C8	−179.03 (17)	C20—S1—C17—C18	1.01 (14)
C2—C7—C8—C9	−2.1 (3)	C20—S1—C17—C16	179.31 (15)
C6—C7—C8—C9	177.69 (17)	C16—C17—C18—N4	−178.77 (15)
C7—C8—C9—N1	−0.7 (3)	S1—C17—C18—N4	−0.5 (2)
C7—C8—C9—C10	179.18 (16)	C16—C17—C18—C19	3.7 (3)
C1—N1—C9—C8	4.3 (2)	S1—C17—C18—C19	−178.11 (17)
C16—N1—C9—C8	−175.35 (17)	C20—N4—C18—C17	−0.5 (2)
C1—N1—C9—C10	−175.59 (15)	C20—N4—C18—C19	177.28 (18)
C16—N1—C9—C10	4.8 (3)	C18—N4—C20—C21	−178.43 (18)
C8—C9—C10—C11	56.7 (2)	C18—N4—C20—S1	1.3 (2)
N1—C9—C10—C11	−123.46 (18)	C17—S1—C20—N4	−1.35 (15)
C8—C9—C10—C15	−122.2 (2)	C17—S1—C20—C21	178.36 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···N2^{i}	0.93	2.62	3.495 (2)	158
C8—H8···N3^{i}	0.93	2.51	3.383 (2)	156

Symmetry code: (i) *x*+1, *y*, *z*.