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Ethyl 2-benzylsulfanyl-7-(2-chlorophenyl)-5-methyl-4,7-dihydro-1,2,4-triazolo[1,5-*a*]pyrimidine-6-carboxylate

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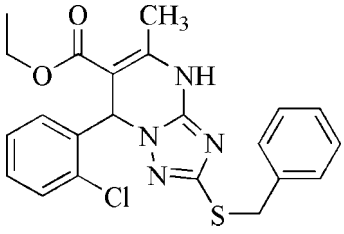
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.143; data-to-parameter ratio = 15.8.

In the title compound, $C_{22}H_{21}ClN_4O_2S$, the bicyclic triazolopyrimidine ring system is nearly planar, and oriented at dihedral angles of 89.45 (3)° with respect to the chlorobenzene ring and 87.03 (3)° with respect to the terminal phenyl ring. In the crystal structure, molecules are linked by π–π stacking interactions between the triazolopyrimidine rings [centroid–centroid distances of 3.88 (1) and 3.63 (1) Å].

Related literature

For general background, see: Fedorova *et al.* (2003). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{22}H_{21}ClN_4O_2S$
M_r = 440.94
Triclinic, $P\overline{1}$
a = 7.5884 (9) Å
b = 10.7303 (12) Å
c = 14.8825 (16) Å
α = 70.655 (2)°
β = 86.097 (2)°
γ = 70.032 (2)°
V = 1073.3 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
7183 measured reflections
4374 independent reflections
3305 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.143
S = 1.07
4374 reflections
277 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2397).

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Fedorova, O. V., Zhidovinova, M. S., Rusinov, G. L. & Ovchinnikova, I. G. (2003). *Russ. Chem. Bull. Int. Ed.* **52**, 1768–1769.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supporting information

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Ethyl 2-benzylsulfanyl-7-(2-chlorophenyl)-5-methyl-4,7-dihydro-1,2,4-triazolo[1,5-*a*]pyrimidine-6-carboxylate

Dan-Dan Song and Qiong Chen

S1. Comment

In recent years, growing attention has been paid to analogues of purines and nucleosides, including azolopyrimidines containing the bridge head nitrogen atom and their dihydro derivatives, among which promising biologically active compounds were found (Fedorova *et al.*, 2003). We synthesized a novel class of ethyl 7-alkylthio-4,7-dihydro-1,2,4-triazolo[1,5-*a*]pyrimidine-6- carboxylate derivatives by three component condensation of 3-amino-5-alkyl- thio-1,2,4-triazoles with aromatic aldehydes and *β*-keto ester. We report herein the crystal structure of one such analogue, a triazolo-pyrimidine derivative, the title compound, (I).

In the molecule of (I), (Fig. 1) the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6), B (N1—N3/C8/C9), C (N3/N4/C9/C10/C12/C13) and D (C14—C19) are, of course, planar. The bicyclic triazolo-pyrimidine ring system (N1—N4/C8—C10/C12/C13) is nearly planar with a maximum deviation of 0.034 (2) Å (for atom C8), and it is oriented with respect to rings A and D at dihedral angles of 87.03 (3)° and 89.45 (3)°, respectively.

In the crystal structure (Fig. 2), molecules are linked by *π*···*π* stacking interactions involving B and C rings of the adjacent molecules with a centroid-centroid distance of 3.88 (1) Å (symmetry code: 1 - *x*, -*y*, 1 - *z*). The adjacent B rings have a centroid-centroid distance of 3.63 (1) %A (symmetry code: 1 - *x*, -*y*, 1 - *z*).

S2. Experimental

For the preparation of the title compound, a mixture of acetylacetic ester (1 mmol), 2-chloro benzaldehyde (1 mmol) and 3-amino-5-benzyllthio-1,2,4 -triazole (1 mmol) in EtOH (3 ml) was added into a microwave tube. The sealed tube was placed in a Smith synthesizer and irradiated at 323 K for 30 min. The reaction mixture was cooled to room temperature, and the precipitate was filtered and recrystallized from ethanol to give the title compound, (I). Single crystals of (I), suitable for X-ray analysis were grown from an acetone solution at 293 K. ^{1}H NMR (CDCl3, 400 MHz): *σ* 10.89(s, 1 H), 7.14–7.41(m, 9 H), 6.84(s, 1H), 4.25(d, 1H), 4.11(d, 1H), 4.02(q,2 H), 2.59(s, 3H),1.08(t, 3H).

S3. Refinement

H atom (for NH) was located in a difference sythesis and refined isotropically [N—H = 0.857 (10) Å and U_{iso}(H) = 0.060 (7) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

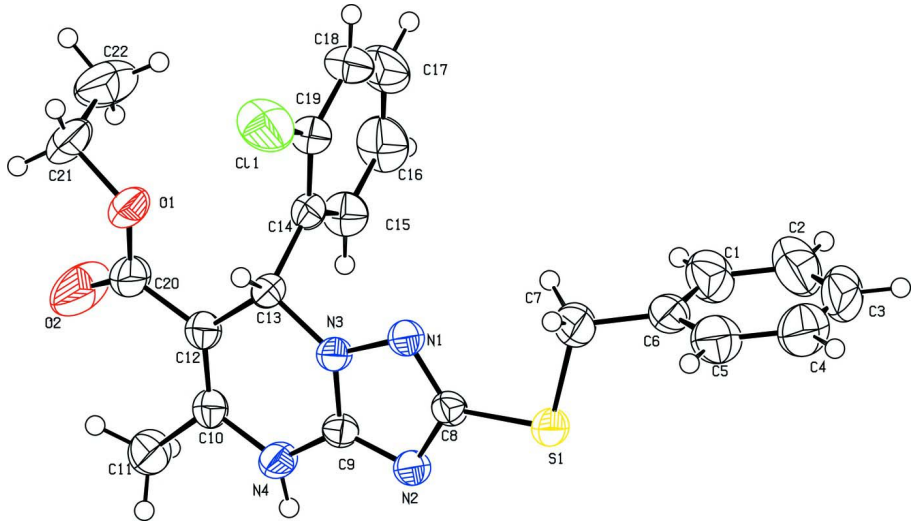

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

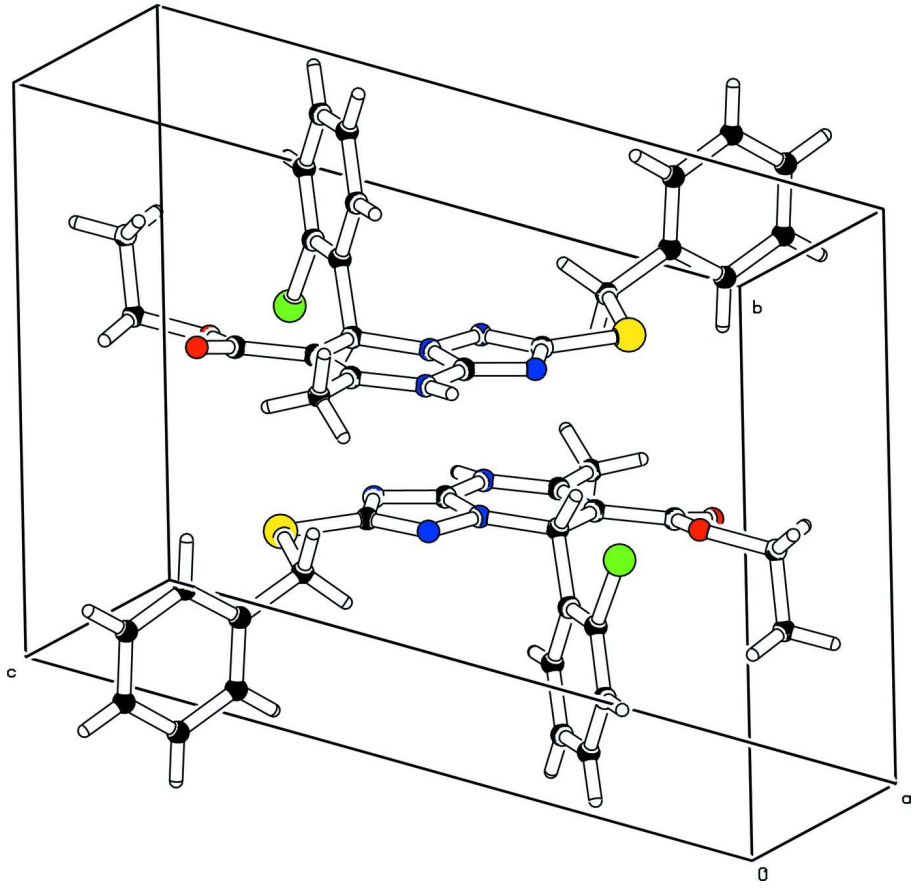

Figure 2

A packing diagram of (I).

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Crystal data

$C_{22}H_{21}ClN_4O_2S$
$M_r = 440.94$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5884$ (9) Å
$b = 10.7303$ (12) Å
$c = 14.8825$ (16) Å
$\alpha = 70.655$ (2)°
$\beta = 86.097$ (2)°
$\gamma = 70.032$ (2)°
$V = 1073.3$ (2) Å^3
$Z = 2$
$F(000) = 460$
$D_x = 1.364$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2807 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.30$ mm^{-1}
$T = 292$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
7183 measured reflections
4374 independent reflections
3305 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.1°$
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 9$
$l = -18 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.143$
$S = 1.07$
4374 reflections
277 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 0.0197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.00615 (8)	0.74321 (8)	0.62526 (6)	0.0777 (3)
S1	0.56904 (7)	0.74334 (6)	0.26984 (4)	0.04454 (19)
O1	0.3353 (2)	0.58296 (17)	0.80362 (10)	0.0535 (4)

O2	0.6149 (3)	0.4999 (3)	0.87766 (13)	0.1116 (10)
N1	0.4468 (2)	0.69605 (17)	0.45014 (11)	0.0355 (4)
N2	0.7612 (2)	0.59780 (17)	0.43894 (11)	0.0348 (4)
N3	0.5383 (2)	0.62604 (17)	0.53959 (11)	0.0341 (4)
N4	0.8411 (2)	0.4984 (2)	0.60747 (12)	0.0427 (5)
H4A	0.9574 (16)	0.473 (2)	0.5949 (17)	0.060 (7)*
C1	0.3133 (4)	1.0947 (3)	0.1521 (2)	0.0676 (7)
H1	0.3380	1.1077	0.2081	0.081*
C2	0.2929 (4)	1.2023 (3)	0.0662 (2)	0.0850 (10)
H2	0.3046	1.2865	0.0646	0.102*
C3	0.2559 (4)	1.1840 (4)	−0.0153 (2)	0.0835 (10)
H3	0.2431	1.2559	−0.0732	0.100*
C4	0.2374 (4)	1.0625 (4)	−0.0136 (2)	0.0831 (10)
H4	0.2119	1.0507	−0.0699	0.100*
C5	0.2567 (4)	0.9554 (3)	0.07242 (19)	0.0660 (7)
H5	0.2417	0.8723	0.0737	0.079*
C6	0.2977 (3)	0.9705 (3)	0.15594 (15)	0.0495 (6)
C7	0.3236 (3)	0.8548 (3)	0.24988 (18)	0.0621 (7)
H7A	0.2458	0.7996	0.2495	0.075*
H7B	0.2859	0.8944	0.3009	0.075*
C8	0.5887 (3)	0.6745 (2)	0.39400 (13)	0.0341 (4)
C9	0.7215 (2)	0.5707 (2)	0.52975 (13)	0.0317 (4)
C10	0.7745 (3)	0.4899 (2)	0.69732 (14)	0.0383 (5)
C11	0.9306 (3)	0.4099 (3)	0.77410 (16)	0.0550 (6)
H11A	0.9949	0.4710	0.7783	0.082*
H11B	1.0175	0.3318	0.7585	0.082*
H11C	0.8785	0.3762	0.8342	0.082*
C12	0.5919 (3)	0.5486 (2)	0.70996 (14)	0.0386 (5)
C13	0.4428 (3)	0.6291 (2)	0.62811 (13)	0.0319 (4)
H13	0.3501	0.5818	0.6358	0.038*
C14	0.3429 (3)	0.7812 (2)	0.62213 (13)	0.0350 (4)
C15	0.4487 (3)	0.8657 (2)	0.61846 (16)	0.0492 (6)
H15	0.5789	0.8280	0.6198	0.059*
C16	0.3652 (5)	1.0036 (3)	0.6129 (2)	0.0687 (8)
H16	0.4385	1.0584	0.6110	0.082*
C17	0.1726 (5)	1.0605 (3)	0.6103 (2)	0.0786 (9)
H17	0.1158	1.1537	0.6070	0.094*
C18	0.0637 (4)	0.9802 (3)	0.61266 (19)	0.0689 (8)
H18	−0.0665	1.0193	0.6098	0.083*
C19	0.1489 (3)	0.8412 (2)	0.61929 (16)	0.0466 (5)
C20	0.5222 (3)	0.5380 (3)	0.80635 (16)	0.0561 (7)
C21	0.2431 (4)	0.6005 (3)	0.88953 (18)	0.0694 (8)
H21A	0.3170	0.5283	0.9451	0.083*
H21B	0.1207	0.5906	0.8897	0.083*
C22	0.2210 (4)	0.7414 (4)	0.8942 (2)	0.0875 (10)
H22A	0.3425	0.7480	0.8998	0.131*
H22B	0.1514	0.7547	0.9486	0.131*
H22C	0.1547	0.8126	0.8372	0.131*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0371 (3)	0.0746 (5)	0.1093 (6)	−0.0209 (3)	−0.0024 (3)	−0.0116 (4)
S1	0.0428 (3)	0.0496 (4)	0.0296 (3)	−0.0035 (2)	−0.0003 (2)	−0.0104 (2)
O1	0.0514 (9)	0.0655 (11)	0.0360 (8)	−0.0116 (8)	0.0119 (7)	−0.0175 (8)
O2	0.0598 (12)	0.191 (3)	0.0364 (11)	0.0100 (14)	−0.0070 (9)	−0.0289 (13)
N1	0.0338 (8)	0.0388 (10)	0.0301 (8)	−0.0072 (7)	−0.0019 (6)	−0.0111 (7)
N2	0.0324 (8)	0.0383 (10)	0.0319 (9)	−0.0079 (7)	−0.0003 (6)	−0.0129 (7)
N3	0.0326 (8)	0.0373 (9)	0.0279 (8)	−0.0050 (7)	−0.0007 (6)	−0.0115 (7)
N4	0.0304 (9)	0.0548 (12)	0.0321 (9)	−0.0044 (8)	0.0003 (7)	−0.0108 (8)
C1	0.0695 (17)	0.0662 (18)	0.0560 (16)	−0.0130 (14)	−0.0143 (13)	−0.0132 (14)
C2	0.081 (2)	0.066 (2)	0.081 (2)	−0.0156 (17)	−0.0161 (17)	0.0031 (17)
C3	0.0563 (17)	0.096 (3)	0.0545 (18)	−0.0082 (17)	−0.0071 (13)	0.0148 (18)
C4	0.0726 (19)	0.110 (3)	0.0423 (16)	−0.0028 (19)	−0.0116 (13)	−0.0199 (17)
C5	0.0603 (16)	0.0753 (19)	0.0547 (16)	−0.0098 (14)	−0.0082 (12)	−0.0232 (14)
C6	0.0347 (11)	0.0571 (15)	0.0402 (12)	−0.0010 (10)	−0.0045 (9)	−0.0087 (11)
C7	0.0415 (12)	0.0680 (17)	0.0490 (14)	−0.0026 (12)	−0.0010 (10)	0.0002 (12)
C8	0.0394 (10)	0.0297 (10)	0.0310 (10)	−0.0069 (8)	−0.0003 (8)	−0.0118 (8)
C9	0.0294 (9)	0.0324 (10)	0.0337 (10)	−0.0097 (8)	0.0005 (8)	−0.0120 (8)
C10	0.0410 (11)	0.0388 (12)	0.0308 (10)	−0.0102 (9)	−0.0009 (8)	−0.0087 (9)
C11	0.0398 (12)	0.0708 (17)	0.0410 (13)	−0.0093 (11)	−0.0071 (9)	−0.0094 (12)
C12	0.0404 (11)	0.0395 (12)	0.0312 (10)	−0.0084 (9)	−0.0010 (8)	−0.0104 (9)
C13	0.0311 (9)	0.0358 (11)	0.0295 (10)	−0.0119 (8)	0.0045 (7)	−0.0118 (8)
C14	0.0390 (10)	0.0359 (11)	0.0291 (10)	−0.0116 (9)	0.0036 (8)	−0.0111 (8)
C15	0.0508 (13)	0.0477 (14)	0.0553 (14)	−0.0207 (11)	0.0022 (11)	−0.0205 (11)
C16	0.097 (2)	0.0515 (16)	0.0724 (19)	−0.0353 (16)	0.0013 (16)	−0.0280 (14)
C17	0.114 (3)	0.0395 (15)	0.0695 (19)	−0.0033 (17)	0.0066 (17)	−0.0253 (14)
C18	0.0657 (17)	0.0520 (16)	0.0658 (17)	0.0071 (13)	0.0101 (13)	−0.0194 (14)
C19	0.0425 (12)	0.0437 (13)	0.0452 (12)	−0.0071 (10)	0.0046 (9)	−0.0123 (10)
C20	0.0497 (13)	0.0652 (16)	0.0344 (12)	−0.0010 (11)	0.0008 (10)	−0.0109 (11)
C21	0.0662 (17)	0.090 (2)	0.0438 (14)	−0.0183 (15)	0.0244 (12)	−0.0237 (14)
C22	0.080 (2)	0.109 (3)	0.082 (2)	−0.0193 (19)	0.0220 (17)	−0.058 (2)

Geometric parameters (Å, º)

Cl1—C19	1.729 (2)	C10—C11	1.512 (3)
N1—C8	1.322 (2)	C11—H11A	0.9600
N1—N3	1.387 (2)	C11—H11B	0.9600
N2—C9	1.321 (2)	C11—H11C	0.9600
N2—C8	1.362 (2)	C12—C20	1.477 (3)
N3—C9	1.332 (2)	C12—C13	1.528 (3)
N3—C13	1.464 (2)	C13—C14	1.521 (3)
N4—C9	1.353 (2)	C13—H13	0.9800
N4—C10	1.382 (2)	C14—C19	1.388 (3)
N4—H4A	0.857 (10)	C14—C15	1.388 (3)
C1—C6	1.360 (4)	C15—C16	1.373 (3)
C1—C2	1.385 (4)	C15—H15	0.9300

C1—H1	0.9300	C16—C17	1.376 (4)
C2—C3	1.354 (4)	C16—H16	0.9300
C2—H2	0.9300	C17—C18	1.374 (4)
C3—C4	1.350 (4)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.381 (3)
C4—C5	1.384 (4)	C18—H18	0.9300
C4—H4	0.9300	C20—O2	1.186 (3)
C5—C6	1.375 (3)	C20—O1	1.331 (3)
C5—H5	0.9300	C21—O1	1.452 (3)
C6—C7	1.502 (3)	C21—C22	1.488 (4)
C7—S1	1.818 (2)	C21—H21A	0.9700
C7—H7A	0.9700	C21—H21B	0.9700
C7—H7B	0.9700	C22—H22A	0.9600
C8—S1	1.744 (2)	C22—H22B	0.9600
C10—C12	1.341 (3)	C22—H22C	0.9600

C8—N1—N3	101.27 (15)	H11B—C11—H11C	109.5
C9—N2—C8	102.11 (15)	C10—C12—C20	121.06 (19)
C9—N3—N1	109.35 (15)	C10—C12—C13	123.50 (18)
C9—N3—C13	127.46 (15)	C20—C12—C13	115.45 (17)
N1—N3—C13	122.90 (14)	N3—C13—C14	108.91 (15)
C9—N4—C10	119.78 (17)	N3—C13—C12	107.18 (15)
C9—N4—H4A	114.4 (16)	C14—C13—C12	113.01 (16)
C10—N4—H4A	125.0 (16)	N3—C13—H13	109.2
C6—C1—C2	121.1 (3)	C14—C13—H13	109.2
C6—C1—H1	119.4	C12—C13—H13	109.2
C2—C1—H1	119.4	C19—C14—C15	117.7 (2)
C3—C2—C1	119.5 (3)	C19—C14—C13	123.08 (19)
C3—C2—H2	120.2	C15—C14—C13	119.19 (18)
C1—C2—H2	120.2	C16—C15—C14	121.4 (2)
C4—C3—C2	120.6 (3)	C16—C15—H15	119.3
C4—C3—H3	119.7	C14—C15—H15	119.3
C2—C3—H3	119.7	C15—C16—C17	119.7 (3)
C3—C4—C5	119.8 (3)	C15—C16—H16	120.2
C3—C4—H4	120.1	C17—C16—H16	120.2
C5—C4—H4	120.1	C18—C17—C16	120.4 (2)
C6—C5—C4	120.6 (3)	C18—C17—H17	119.8
C6—C5—H5	119.7	C16—C17—H17	119.8
C4—C5—H5	119.7	C17—C18—C19	119.5 (3)
C1—C6—C5	118.3 (2)	C17—C18—H18	120.2
C1—C6—C7	120.0 (2)	C19—C18—H18	120.2
C5—C6—C7	121.7 (3)	C18—C19—C14	121.2 (2)
C6—C7—S1	109.29 (16)	C18—C19—Cl1	117.8 (2)
C6—C7—H7A	109.8	C14—C19—Cl1	120.93 (17)
S1—C7—H7A	109.8	O2—C20—O1	122.7 (2)
C6—C7—H7B	109.8	O2—C20—C12	126.4 (2)
S1—C7—H7B	109.8	O1—C20—C12	110.83 (19)
H7A—C7—H7B	108.3	O1—C21—C22	110.2 (2)

N1—C8—N2	115.88 (17)	O1—C21—H21A	109.6
N1—C8—S1	124.52 (15)	C22—C21—H21A	109.6
N2—C8—S1	119.54 (14)	O1—C21—H21B	109.6
N2—C9—N3	111.39 (16)	C22—C21—H21B	109.6
N2—C9—N4	128.22 (17)	H21A—C21—H21B	108.1
N3—C9—N4	120.38 (17)	C21—C22—H22A	109.5
C12—C10—N4	121.53 (18)	C21—C22—H22B	109.5
C12—C10—C11	126.76 (19)	H22A—C22—H22B	109.5
N4—C10—C11	111.71 (18)	C21—C22—H22C	109.5
C10—C11—H11A	109.5	H22A—C22—H22C	109.5
C10—C11—H11B	109.5	H22B—C22—H22C	109.5
H11A—C11—H11B	109.5	C20—O1—C21	117.94 (19)
C10—C11—H11C	109.5	C8—S1—C7	101.13 (10)
H11A—C11—H11C	109.5		

C8—N1—N3—C9	0.3 (2)	C9—N3—C13—C12	−3.3 (3)
C8—N1—N3—C13	174.42 (17)	N1—N3—C13—C12	−176.31 (16)
C6—C1—C2—C3	0.3 (5)	C10—C12—C13—N3	0.6 (3)
C1—C2—C3—C4	0.5 (5)	C20—C12—C13—N3	−179.11 (18)
C2—C3—C4—C5	−0.1 (5)	C10—C12—C13—C14	−119.4 (2)
C3—C4—C5—C6	−1.1 (4)	C20—C12—C13—C14	60.9 (2)
C2—C1—C6—C5	−1.5 (4)	N3—C13—C14—C19	113.7 (2)
C2—C1—C6—C7	179.0 (2)	C12—C13—C14—C19	−127.3 (2)
C4—C5—C6—C1	1.9 (4)	N3—C13—C14—C15	−65.7 (2)
C4—C5—C6—C7	−178.6 (2)	C12—C13—C14—C15	53.3 (2)
C1—C6—C7—S1	−91.0 (3)	C19—C14—C15—C16	0.5 (3)
C5—C6—C7—S1	89.5 (3)	C13—C14—C15—C16	179.9 (2)
N3—N1—C8—N2	−0.1 (2)	C14—C15—C16—C17	−0.4 (4)
N3—N1—C8—S1	−177.04 (14)	C15—C16—C17—C18	−0.4 (4)
C9—N2—C8—N1	−0.2 (2)	C16—C17—C18—C19	1.1 (4)
C9—N2—C8—S1	176.97 (14)	C17—C18—C19—C14	−1.0 (4)
C8—N2—C9—N3	0.3 (2)	C17—C18—C19—Cl1	178.3 (2)
C8—N2—C9—N4	−179.2 (2)	C15—C14—C19—C18	0.3 (3)
N1—N3—C9—N2	−0.4 (2)	C13—C14—C19—C18	−179.2 (2)
C13—N3—C9—N2	−174.21 (17)	C15—C14—C19—Cl1	−179.04 (16)
N1—N3—C9—N4	179.18 (18)	C13—C14—C19—Cl1	1.5 (3)
C13—N3—C9—N4	5.4 (3)	C10—C12—C20—O2	12.7 (4)
C10—N4—C9—N2	175.17 (19)	C13—C12—C20—O2	−167.6 (3)
C10—N4—C9—N3	−4.3 (3)	C10—C12—C20—O1	−169.8 (2)
C9—N4—C10—C12	1.9 (3)	C13—C12—C20—O1	9.9 (3)
C9—N4—C10—C11	−177.66 (19)	O2—C20—O1—C21	7.1 (4)
N4—C10—C12—C20	179.6 (2)	C12—C20—O1—C21	−170.5 (2)
C11—C10—C12—C20	−1.0 (4)	C22—C21—O1—C20	85.4 (3)
N4—C10—C12—C13	−0.1 (3)	N1—C8—S1—C7	5.3 (2)
C11—C10—C12—C13	179.4 (2)	N2—C8—S1—C7	−171.56 (17)
C9—N3—C13—C14	119.3 (2)	C6—C7—S1—C8	154.37 (19)
N1—N3—C13—C14	−53.7 (2)		