Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-Bromo-3,3-dibutyl-8-methoxy-2,3-dihydro-1,5-benzothiazepin-4(5*H*)-one

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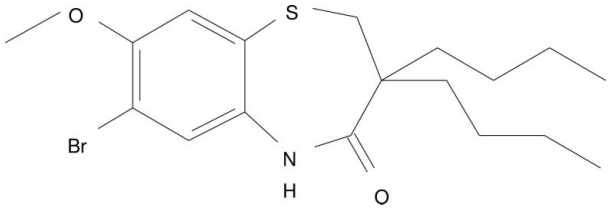
Received 7 May 2013; accepted 14 May 2013

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.006 Å; R factor = 0.050; wR factor = 0.187; data-to-parameter ratio = 22.1.

In the title compound $C_{18}H_{26}BrNO_2S$, the thiazepine ring adopts a boat conformation. The dihedral angle between the mean planes through the benzene ring and the four C atoms making up the basal plane of the boat is 35.8 (2)°. In the crystal, inversion dimers linked by pairs of N—H···O hydrogen bonds generate $R_2^2(8)$ loops.

Related literature

For reference bond lengths, see: Allen *et al.* (1987). For background to the uses of this class of compounds, see: Fedi *et al.* (2008); Ganesh *et al.* (2011); Riedel *et al.* (2007).



Experimental

Crystal data

$C_{18}H_{26}BrNO_2S$
M_r = 400.30
Monoclinic, $P2_1/n$
a = 7.7844 (18) Å
b = 11.251 (2) Å
c = 22.039 (6) Å
β = 98.199 (8)°
V = 1910.5 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.27 mm^{-1}
T = 100 K
0.32 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
16056 measured reflections
4662 independent reflections
2750 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.141
S = 1.03
4662 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N14—H14···O15^{i}	0.86	2.13	2.985 (3)	175

Symmetry code: (i) $-x+1, -y+1, -z+2$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *Mercury*.

MM thanks the IOE and the University of Mysore for the award of a fellowship and research grants. The data collection was performed at the Solid Sate and Structural Chemistry Unit, IISC.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7081).

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supplementary materials

Acta Cryst. (2013). E**69**, o1129 [doi:10.1107/S1600536813013238]

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Comment

The title compound $C_{18}H_{25}Br_NO_2S$, was synthesized from 3,3-dibutyl-2,3- dihydro-8-methoxybenzo[*b*][1,4]thiazepin-4(5*H*)-one. The molecule is a bicyclic structure with one aromatic ring fused to a seven membered ring, on which two heteroatoms are present. The derivatives of this molecule able to provide high affinity ligands for more than one type of the receptor (Fedi *et al.*, 2008). The compound is mainly used to treat schizophrenia and also find applications as neuroleptics, antidepressants, antihistaminic (Ganesh *et al.*, 2011; Riedel *et al.*, 2007). The N14—C13 bond is shorter than an usual N—C single bond [1.356 Å compared to 1.416 Å (Allen *et al.* 1987)]. The atoms C5, C6, C11 and C12 present in the central thiazepine ring forms a basal plane and the S10 atom as the bow, representing the boat conformation of thiazepine ring.

Experimental

3,3-dibutyl-2,3-dihydro-8-methoxybenzo[*b*][1,4]thiazepin-4(5*H*)-one in dichloromethane, acetonitrile, cooled to 5°C and added *N*-bromosuccinimide over a period of 15 min. Then reaction mixture was brought to room temperature, stirred for 2 h and again cooled to 5°C, then *N*-bromosuccinimide is added at 5°C, cooled to -5°C for 1 h, filtered, washed with cold acetonitrile and then dried in vacuum and product was recrystallized from acetonitrile solution to yield light brown blocks.

Refinement

All hydrogen atoms were located geometrically with C—H = 0.93–0.97 Å and allowed to ride on their parent atoms with U_{iso}(H) = 1.2U_{eq}(aromatic C).

Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2006).

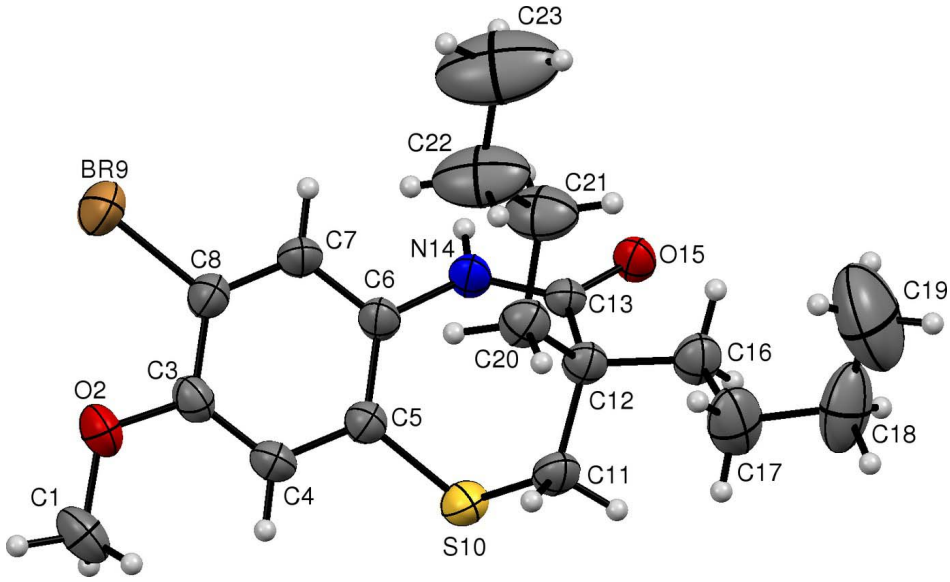

Figure 1

View of the title molecule with 50% probability ellipsoids.

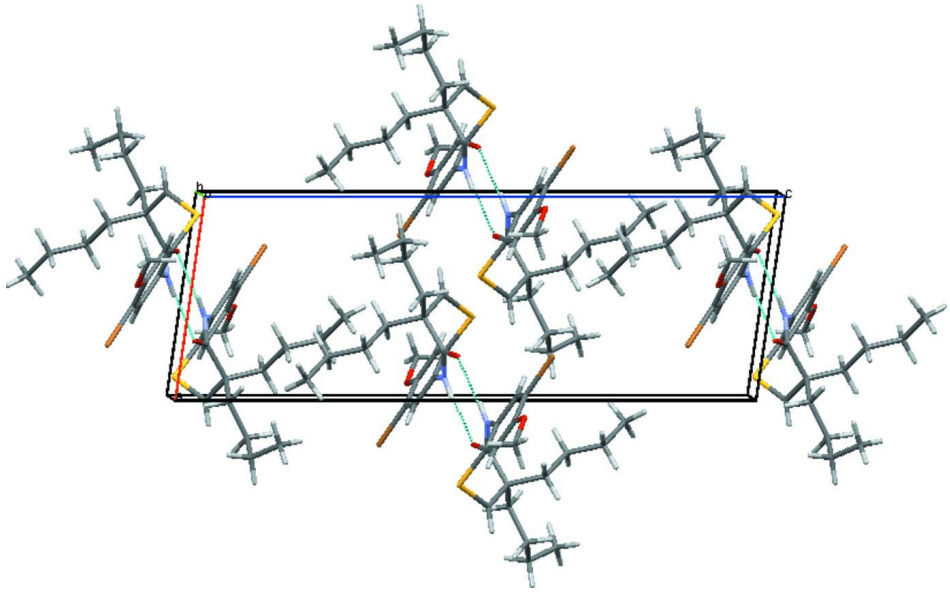

Figure 2

Packing diagram of molecule, viewed along the crystallographic *b* axis.

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Crystal data

$C_{18}H_{26}BrNO_2S$
$M_r = 400.30$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.7844\ (18)$ Å
$b = 11.251\ (2)$ Å
$c = 22.039\ (6)$ Å
$\beta = 98.199\ (8)°$
$V = 1910.5\ (8)$ Å^3
$Z = 4$
$F(000) = 832$
$D_x = 1.392$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4662 reflections

θ = 2.0–28.3°
μ = 2.27 mm^{-1}
T = 100 K

Block, light brown
0.32 × 0.20 × 0.20 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0839 pixels mm^{-1}
ω scans
16056 measured reflections

4662 independent reflections
2750 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 28.3°, θ_{min} = 2.0°
h = −10→8
k = −14→9
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.141
S = 1.03
4662 reflections
212 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
$w = 1/[\sigma^2(F_o^2) + (0.1275P)^2 + 0.4493P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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 esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
Br9	0.72841 (5)	0.01588 (4)	0.86915 (2)	0.0731 (2)
S10	0.09376 (11)	0.21269 (7)	0.99530 (4)	0.0494 (3)
O2	0.4327 (3)	−0.12202 (18)	0.90398 (11)	0.0548 (8)
O15	0.2816 (3)	0.53731 (17)	0.97428 (10)	0.0420 (7)
N14	0.3916 (3)	0.35886 (16)	0.95950 (10)	0.0418 (8)
C1	0.3047 (3)	−0.20519 (16)	0.91627 (10)	0.0621 (15)
C3	0.4122 (4)	−0.0060 (2)	0.91890 (15)	0.0399 (10)
C4	0.2747 (4)	0.0385 (3)	0.94491 (15)	0.0412 (10)
C5	0.2640 (4)	0.1590 (2)	0.95831 (14)	0.0383 (10)
C6	0.3919 (3)	0.2370 (2)	0.94450 (14)	0.0377 (9)
C7	0.5283 (4)	0.1922 (3)	0.91780 (15)	0.0424 (10)
C8	0.5387 (4)	0.0733 (3)	0.90492 (15)	0.0435 (10)
C11	−0.0156 (4)	0.3122 (3)	0.93772 (15)	0.0460 (10)
C12	0.0909 (4)	0.4072 (3)	0.90861 (14)	0.0386 (9)
C13	0.2596 (3)	0.4382 (2)	0.95076 (14)	0.0353 (9)

C16	−0.0182 (4)	0.5206 (3)	0.89941 (17)	0.0481 (11)
C17	−0.1953 (5)	0.5099 (3)	0.8591 (2)	0.0743 (16)
C18	−0.2889 (6)	0.6281 (5)	0.8496 (2)	0.0915 (19)
C19	−0.2269 (11)	0.7005 (6)	0.8047 (4)	0.165 (4)
C20	0.1333 (4)	0.3605 (3)	0.84640 (14)	0.0467 (11)
C21	0.2456 (6)	0.4427 (4)	0.81384 (18)	0.0743 (16)
C22	0.2854 (7)	0.3940 (6)	0.7533 (2)	0.105 (2)
C23	0.3966 (11)	0.4756 (7)	0.7214 (3)	0.165 (4)
H1A	0.30480	−0.21090	0.95970	0.0940*
H1B	0.33020	−0.28160	0.90040	0.0940*
H1C	0.19260	−0.17920	0.89700	0.0940*
H4	0.18770	−0.01270	0.95360	0.0490*
H7	0.61460	0.24340	0.90840	0.0510*
H11A	−0.07390	0.26350	0.90470	0.0550*
H11B	−0.10520	0.35340	0.95590	0.076 (12)*
H14	0.48930	0.38680	0.97670	0.061 (10)*
H16A	0.04900	0.58050	0.88150	0.0580*
H16B	−0.03720	0.54940	0.93940	0.053 (10)*
H17A	−0.17880	0.47760	0.81960	0.0890*
H17B	−0.26710	0.45470	0.87810	0.0890*
H18A	−0.41170	0.61340	0.83740	0.1100*
H18B	−0.27580	0.67080	0.88820	0.1100*
H19A	−0.12380	0.74130	0.82270	0.2470*
H19B	−0.31420	0.75760	0.78950	0.2470*
H19C	−0.20070	0.65160	0.77150	0.2470*
H20A	0.19210	0.28460	0.85320	0.0560*
H20B	0.02520	0.34660	0.81960	0.0560*
H21A	0.18690	0.51850	0.80660	0.0890*
H21B	0.35400	0.45680	0.84050	0.0890*
H22A	0.34410	0.31820	0.76050	0.1260*
H22B	0.17710	0.38000	0.72660	0.1260*
H23A	0.32730	0.54030	0.70310	0.2480*
H23B	0.44400	0.43230	0.69000	0.2480*
H23C	0.48940	0.50610	0.75050	0.2480*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br9	0.0585 (3)	0.0543 (3)	0.1145 (4)	0.0039 (2)	0.0399 (2)	−0.0172 (2)
S10	0.0463 (5)	0.0452 (5)	0.0608 (6)	−0.0023 (3)	0.0220 (4)	−0.0027 (4)
O2	0.0634 (15)	0.0289 (11)	0.0748 (16)	−0.0011 (10)	0.0188 (12)	−0.0065 (11)
O15	0.0329 (11)	0.0317 (11)	0.0600 (14)	−0.0040 (8)	0.0020 (10)	−0.0114 (10)
N14	0.0289 (13)	0.0310 (13)	0.0642 (17)	−0.0052 (10)	0.0019 (12)	−0.0106 (12)
C1	0.077 (3)	0.0328 (18)	0.076 (3)	−0.0101 (17)	0.009 (2)	−0.0023 (17)
C3	0.0439 (17)	0.0286 (15)	0.0460 (19)	−0.0026 (12)	0.0022 (14)	−0.0037 (13)
C4	0.0390 (16)	0.0333 (16)	0.052 (2)	−0.0074 (12)	0.0092 (14)	−0.0011 (14)
C5	0.0352 (16)	0.0348 (16)	0.0456 (18)	−0.0019 (12)	0.0082 (13)	−0.0042 (13)
C6	0.0296 (14)	0.0308 (15)	0.0513 (19)	−0.0023 (11)	0.0010 (13)	−0.0054 (13)
C7	0.0292 (15)	0.0367 (16)	0.062 (2)	−0.0051 (12)	0.0090 (14)	−0.0041 (15)
C8	0.0360 (16)	0.0391 (17)	0.057 (2)	0.0014 (13)	0.0125 (14)	−0.0067 (15)

C11	0.0302 (15)	0.0442 (17)	0.064 (2)	−0.0063 (13)	0.0080 (15)	−0.0109 (16)
C12	0.0308 (15)	0.0375 (16)	0.0469 (18)	−0.0047 (12)	0.0033 (13)	−0.0078 (14)
C13	0.0297 (14)	0.0309 (15)	0.0464 (18)	−0.0038 (11)	0.0097 (13)	−0.0034 (13)
C16	0.0361 (17)	0.0452 (18)	0.061 (2)	−0.0002 (13)	−0.0003 (16)	−0.0098 (16)
C17	0.050 (2)	0.064 (3)	0.099 (3)	0.0067 (18)	−0.023 (2)	−0.008 (2)
C18	0.072 (3)	0.098 (4)	0.093 (3)	0.040 (3)	−0.028 (3)	−0.029 (3)
C19	0.200 (8)	0.089 (4)	0.193 (8)	0.039 (5)	−0.013 (7)	0.019 (5)
C20	0.0398 (17)	0.0490 (19)	0.050 (2)	−0.0056 (14)	0.0020 (14)	−0.0106 (15)
C21	0.083 (3)	0.088 (3)	0.055 (2)	−0.022 (2)	0.021 (2)	−0.006 (2)
C22	0.108 (4)	0.159 (5)	0.052 (3)	−0.046 (4)	0.026 (3)	−0.017 (3)
C23	0.151 (7)	0.270 (10)	0.081 (4)	−0.078 (6)	0.037 (4)	−0.028 (5)

Geometric parameters (Å, º)

Br9—C8	1.885 (3)	C1—H1A	0.9600
S10—C5	1.759 (3)	C1—H1B	0.9600
S10—C11	1.811 (3)	C1—H1C	0.9600
O2—C1	1.421 (3)	C4—H4	0.9300
O2—C3	1.361 (3)	C7—H7	0.9300
O15—C13	1.231 (3)	C11—H11A	0.9700
N14—C6	1.410 (3)	C11—H11B	0.9700
N14—C13	1.354 (3)	C16—H16A	0.9700
N14—H14	0.8600	C16—H16B	0.9700
C3—C4	1.378 (4)	C17—H17A	0.9700
C3—C8	1.395 (4)	C17—H17B	0.9700
C4—C5	1.393 (4)	C18—H18A	0.9700
C5—C6	1.393 (4)	C18—H18B	0.9700
C6—C7	1.381 (4)	C19—H19A	0.9600
C7—C8	1.372 (5)	C19—H19B	0.9600
C11—C12	1.547 (5)	C19—H19C	0.9600
C12—C13	1.537 (4)	C20—H20A	0.9700
C12—C16	1.530 (5)	C20—H20B	0.9700
C12—C20	1.547 (4)	C21—H21A	0.9700
C16—C17	1.535 (5)	C21—H21B	0.9700
C17—C18	1.517 (6)	C22—H22A	0.9700
C18—C19	1.418 (9)	C22—H22B	0.9700
C20—C21	1.521 (6)	C23—H23A	0.9600
C21—C22	1.515 (6)	C23—H23B	0.9600
C22—C23	1.503 (10)	C23—H23C	0.9600
C5—S10—C11	101.39 (14)	S10—C11—H11B	107.00
C1—O2—C3	118.4 (2)	C12—C11—H11A	107.00
C6—N14—C13	129.4 (2)	C12—C11—H11B	107.00
C13—N14—H14	115.00	H11A—C11—H11B	107.00
C6—N14—H14	115.00	C12—C16—H16A	108.00
C4—C3—C8	118.3 (3)	C12—C16—H16B	108.00
O2—C3—C4	125.0 (3)	C17—C16—H16A	108.00
O2—C3—C8	116.7 (3)	C17—C16—H16B	108.00
C3—C4—C5	121.0 (3)	H16A—C16—H16B	107.00
S10—C5—C4	120.3 (2)	C16—C17—H17A	109.00

S10—C5—C6	119.61 (18)	C16—C17—H17B	109.00
C4—C5—C6	120.1 (3)	C18—C17—H17A	109.00
N14—C6—C5	122.4 (2)	C18—C17—H17B	109.00
C5—C6—C7	118.7 (2)	H17A—C17—H17B	108.00
N14—C6—C7	118.8 (2)	C17—C18—H18A	109.00
C6—C7—C8	121.1 (3)	C17—C18—H18B	109.00
Br9—C8—C3	119.5 (2)	C19—C18—H18A	109.00
Br9—C8—C7	119.6 (2)	C19—C18—H18B	109.00
C3—C8—C7	120.9 (3)	H18A—C18—H18B	108.00
S10—C11—C12	119.4 (2)	C18—C19—H19A	110.00
C11—C12—C20	109.1 (3)	C18—C19—H19B	109.00
C13—C12—C16	107.5 (3)	C18—C19—H19C	109.00
C13—C12—C20	109.9 (2)	H19A—C19—H19B	109.00
C16—C12—C20	110.5 (3)	H19A—C19—H19C	109.00
C11—C12—C16	108.1 (3)	H19B—C19—H19C	110.00
C11—C12—C13	111.6 (2)	C12—C20—H20A	109.00
O15—C13—C12	121.0 (2)	C12—C20—H20B	109.00
O15—C13—N14	118.7 (2)	C21—C20—H20A	109.00
N14—C13—C12	120.1 (2)	C21—C20—H20B	109.00
C12—C16—C17	116.6 (3)	H20A—C20—H20B	108.00
C16—C17—C18	112.7 (3)	C20—C21—H21A	109.00
C17—C18—C19	113.3 (5)	C20—C21—H21B	109.00
C12—C20—C21	114.9 (3)	C22—C21—H21A	109.00
C20—C21—C22	113.5 (4)	C22—C21—H21B	109.00
C21—C22—C23	113.3 (5)	H21A—C21—H21B	108.00
O2—C1—H1A	109.00	C21—C22—H22A	109.00
O2—C1—H1B	109.00	C21—C22—H22B	109.00
O2—C1—H1C	109.00	C23—C22—H22A	109.00
H1A—C1—H1B	109.00	C23—C22—H22B	109.00
H1A—C1—H1C	109.00	H22A—C22—H22B	108.00
H1B—C1—H1C	110.00	C22—C23—H23A	109.00
C3—C4—H4	119.00	C22—C23—H23B	109.00
C5—C4—H4	119.00	C22—C23—H23C	110.00
C6—C7—H7	120.00	H23A—C23—H23B	109.00
C8—C7—H7	119.00	H23A—C23—H23C	110.00
S10—C11—H11A	107.00	H23B—C23—H23C	109.00

C11—S10—C5—C4	−117.4 (3)	C5—C6—C7—C8	0.0 (5)
C11—S10—C5—C6	65.0 (3)	C6—C7—C8—Br9	−179.4 (2)
C5—S10—C11—C12	−51.1 (3)	C6—C7—C8—C3	−0.5 (5)
C1—O2—C3—C4	−0.6 (5)	S10—C11—C12—C13	−23.9 (4)
C1—O2—C3—C8	−178.7 (3)	S10—C11—C12—C16	−142.0 (2)
C13—N14—C6—C5	−47.0 (4)	S10—C11—C12—C20	97.8 (3)
C13—N14—C6—C7	136.2 (3)	C11—C12—C13—O15	−113.0 (3)
C6—N14—C13—O15	170.9 (3)	C11—C12—C13—N14	71.2 (3)
C6—N14—C13—C12	−13.2 (4)	C16—C12—C13—O15	5.4 (4)
O2—C3—C4—C5	−179.6 (3)	C16—C12—C13—N14	−170.4 (3)
C8—C3—C4—C5	−1.5 (5)	C20—C12—C13—O15	125.7 (3)
O2—C3—C8—Br9	−1.6 (4)	C20—C12—C13—N14	−50.0 (4)

O2—C3—C8—C7	179.5 (3)	C11—C12—C16—C17	−58.6 (4)
C4—C3—C8—Br9	−179.9 (2)	C13—C12—C16—C17	−179.2 (3)
C4—C3—C8—C7	1.2 (5)	C20—C12—C16—C17	60.8 (4)
C3—C4—C5—S10	−176.5 (3)	C11—C12—C20—C21	−177.2 (3)
C3—C4—C5—C6	1.1 (5)	C13—C12—C20—C21	−54.5 (4)
S10—C5—C6—N14	0.5 (4)	C16—C12—C20—C21	64.1 (4)
S10—C5—C6—C7	177.3 (2)	C12—C16—C17—C18	−176.6 (3)
C4—C5—C6—N14	−177.2 (3)	C16—C17—C18—C19	79.1 (6)
C4—C5—C6—C7	−0.3 (5)	C12—C20—C21—C22	179.7 (3)
N14—C6—C7—C8	177.0 (3)	C20—C21—C22—C23	−179.9 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N14—H14···O15^{i}	0.86	2.13	2.985 (3)	175
C11—H11*B*···O15^{ii}	0.97	2.52	3.473 (4)	166

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