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1,4-Bis[4-(methoxycarbonyl)benzyl]-1*H*-1,2,4-triazol-4-ium bromide

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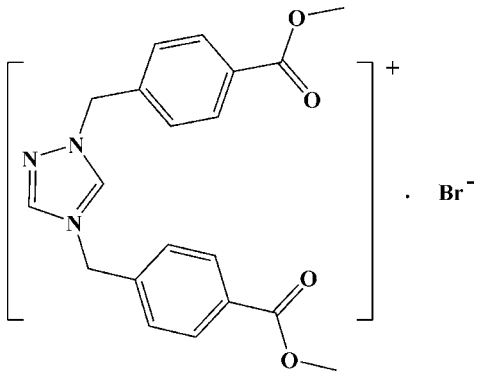
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.069; data-to-parameter ratio = 10.6.

In the title salt, $C_{20}H_{20}N_3O_4^+\cdot Br^-$, the dihedral angle between the benzene rings is 8.69 (16)°, and those between the benzene rings and the triazole ring are 69.98 (18) and 72.17 (18)°. In the crystal, C—H···Br hydrogen bonds link the cations and anions into chains along the c axis.

Related literature

For general background to triazole derivatives, see: Zanardi *et al.* (2011). For a related structure, see: Huang *et al.* (2010).



Experimental

Crystal data

$C_{20}H_{20}N_3O_4^+\cdot Br^-$
M_r = 446.30
Orthorhombic, $Pca2_1$
a = 33.6880 (15) Å
b = 4.7962 (3) Å
c = 12.3337 (6) Å
V = 1992.81 (18) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.08 mm^{-1}
T = 173 K
0.40 × 0.32 × 0.31 mm

Data collection

Oxford Diffraction Xcalibur Atlas Gemini Ultra diffractometer
Absorption correction: multi-scan (*ABSPACK* in *CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min} = 0.372, T_{max} = 0.449
6375 measured reflections
2709 independent reflections
2541 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.069
S = 1.05
2709 reflections
255 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 840 Friedel pairs
Flack parameter: 0.021 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···Br1	0.95	2.61	3.461 (3)	149
C3—H3A···Br1	0.99	2.91	3.795 (4)	149
C2—H2···Br1^{i}	0.95	2.75	3.657 (3)	161

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); 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: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5263).

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supporting information

Acta Cryst. (2012). E**68**, o1553 [doi:10.1107/S1600536812016728]

1,4-Bis[4-(methoxycarbonyl)benzyl]-1*H*-1,2,4-triazol-4-ium bromide

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S1. Comment

1*H*-1,2,4-Triazole, like imidazole and benzimidazole, can be *N*-alkylated to form *N*-heterocyclic carbine (Zanardi *et al.*, 2011).

In an earlier report, we presented a *N*-heterocyclic benzimidazole derivative. The crystal structure consists of infinite chains connected *via* C—H···Br and C—H···O hydrogen bonds; it also shows $\pi\cdots\pi$ stacking interactions (Huang *et al.*, 2010).

In this work, we report the structure of a triazole-based *N*-heterocyclic carbene, 1,4-bis[4-(methoxycarbonyl)-benzyl]-1*H*-1,2,4-triazolium bromide (Fig. 1).

In the crystal structure, the dihedral angles between the triazole ring system and the two (C4–C9) and (C13–C18) benzene rings are 69.98 (18) ° and 72.17 (18) °, respectively; the dihedral angle between the two benzene rings is 8.69 (16) °.

The bromide anions and cations form infinite hydrogen bonding chains along the *c*-axis *via* C—H···Br hydrogen bonds between the bromide anions and carbineen atoms of triazole ring and ethylene linkage (Fig. 2, Table 1).

S2. Experimental

4-(Methoxycarbonyl)benzyl bromide (2.28 g, 10.0 mmol) was slowly added to a solution of 1*H*-1,2,4-triazole (0.35 g, 5.0 mmol) in acetonitrile (25 ml) and the resulting mixture was stirred under reflux for 8 h.

The solvent was evaporated under reduced pressure. The solid residue was recrystallized in methanol, and colorless block crystals were obtained after few days, yield 1.42 g, 63.5%.

Elemental analysis, calcd (%) for $C_{20}H_{20}N_3BrO_4$: C 53.82, H 4.52, N 9.42; found(%): C 53.80, H 4.60, N 9.41.

The FAB mass spectrum showed tje ions at 447.

S3. Refinement

The C-bound H atoms were positioned geometrically and were included in the refinement in the riding-model approximation, with distances 0.98 (CH_3), 0.99 (CH_2) and 0.95 Å (aromatic and triazole); $U_{iso}(H) = xU_{eq}$(attached atom), where x = 1.5 for methyl C and 1.2 for all other C.

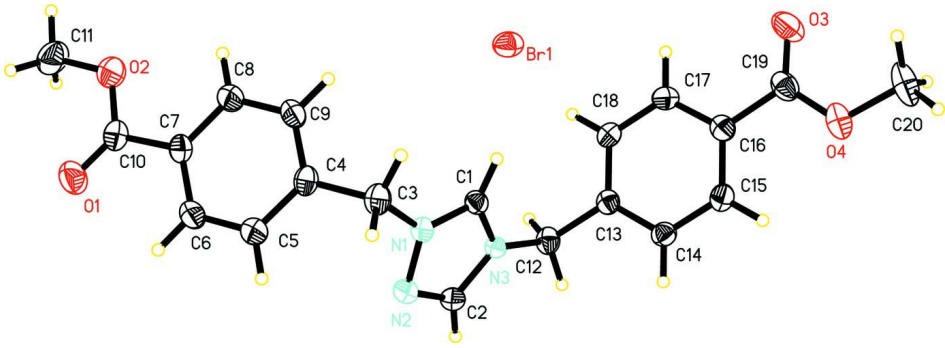

Figure 1

Perspective view showing 30% probability displacement ellipsoids and the atom-numbering scheme.

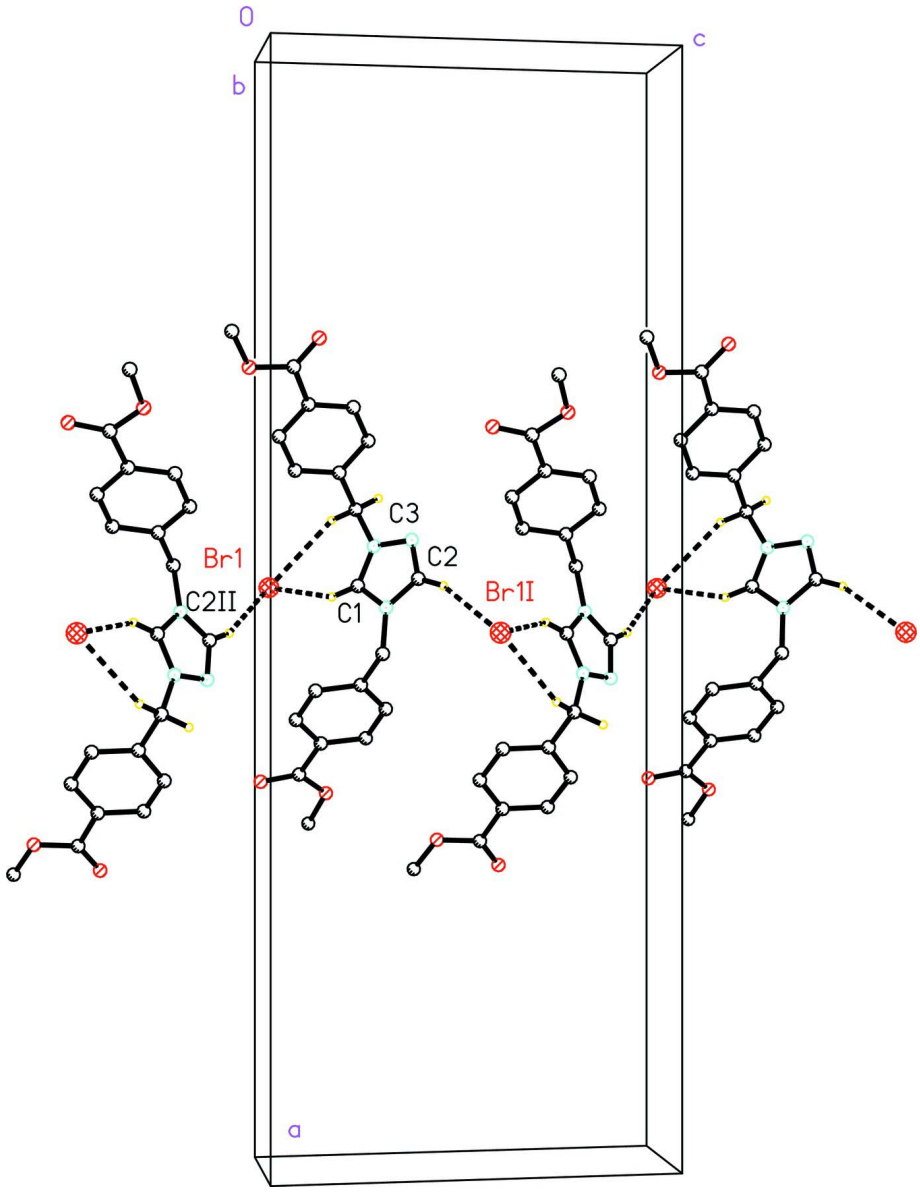

Figure 2

Crystal packing of the title compound. Dashed lines indicate hydrogen bonds. Symmetry: I = -*x* + 1, -*y* + 1, *z* + 1/2; II = -*x* + 1, -*y* + 2, *z* + 1/2. H atoms not involved in the hydrogen bond interactions have been omitted.

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Crystal data

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M_r = 446.30
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a = 33.6880 (15) Å
b = 4.7962 (3) Å
c = 12.3337 (6) Å
V = 1992.81 (18) Å^3
Z = 4
F(000) = 912
D_x = 1.488 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 3691 reflections
θ = 3.6–66.9°
μ = 3.08 mm^{-1}
T = 173 K
Block, colorless
0.40 × 0.32 × 0.31 mm

Data collection

Oxford Diffraction Xcalibur Atlas Gemini Ultra diffractometer
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.5058 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (ABSPACK in *CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min} = 0.372, T_{max} = 0.449
6375 measured reflections
2709 independent reflections
2541 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 66.9°, θ_{min} = 4.4°
h = −40→39
k = −5→4
l = −11→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.069
S = 1.05
2709 reflections
255 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 0.0837P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack (1983), 840 Friedel pairs
Absolute structure parameter: 0.021 (18)

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}
C1	0.47864 (8)	0.6564 (6)	0.2417 (3)	0.0375 (7)
H1	0.4887	0.7596	0.1819	0.045*
C2	0.47240 (9)	0.3718 (7)	0.3756 (3)	0.0452 (7)
H2	0.4788	0.2350	0.4285	0.054*
C3	0.40894 (9)	0.8422 (7)	0.2458 (3)	0.0480 (8)
H3A	0.4184	0.9793	0.1917	0.058*
H3B	0.3980	0.9465	0.3083	0.058*
C4	0.37667 (8)	0.6644 (6)	0.1961 (3)	0.0441 (7)
C5	0.34867 (10)	0.5364 (9)	0.2611 (3)	0.0554 (9)
H5	0.3490	0.5665	0.3373	0.067*
C6	0.32036 (11)	0.3655 (9)	0.2160 (3)	0.0599 (10)
H6	0.3017	0.2741	0.2616	0.072*
C7	0.31867 (9)	0.3249 (7)	0.1051 (3)	0.0450 (7)

C8	0.34607 (8)	0.4583 (7)	0.0390 (4)	0.0538 (7)
H8	0.3449	0.4351	−0.0374	0.065*
C9	0.37509 (10)	0.6255 (8)	0.0851 (3)	0.0533 (9)
H9	0.3941	0.7143	0.0399	0.064*
C10	0.28761 (9)	0.1331 (7)	0.0608 (4)	0.0518 (10)
C11	0.26013 (14)	−0.0757 (11)	−0.0946 (4)	0.0807 (13)
H11A	0.2335	−0.0263	−0.0690	0.121*
H11B	0.2662	−0.2681	−0.0735	0.121*
H11C	0.2612	−0.0592	−0.1737	0.121*
C12	0.53934 (10)	0.3639 (7)	0.2875 (3)	0.0456 (8)
H12A	0.5389	0.2054	0.2361	0.055*
H12B	0.5492	0.2936	0.3580	0.055*
C13	0.56784 (9)	0.5850 (7)	0.2453 (3)	0.0389 (7)
C14	0.59021 (9)	0.7440 (7)	0.3159 (3)	0.0421 (7)
H14	0.5868	0.7241	0.3919	0.051*
C15	0.61770 (9)	0.9330 (7)	0.2758 (3)	0.0454 (7)
H15	0.6334	1.0398	0.3246	0.054*
C16	0.62246 (8)	0.9668 (7)	0.1643 (3)	0.0428 (7)
C17	0.59997 (10)	0.8069 (8)	0.0951 (3)	0.0521 (8)
H17	0.6030	0.8288	0.0190	0.063*
C18	0.57294 (9)	0.6139 (8)	0.1348 (3)	0.0475 (7)
H18	0.5580	0.5021	0.0861	0.057*
C19	0.65221 (11)	1.1610 (8)	0.1181 (4)	0.0541 (10)
C20	0.70101 (11)	1.5049 (8)	0.1569 (5)	0.0781 (14)
H20A	0.7055	1.6461	0.2130	0.117*
H20B	0.6921	1.5960	0.0901	0.117*
H20C	0.7258	1.4045	0.1429	0.117*
N1	0.44256 (8)	0.6675 (5)	0.2823 (2)	0.0398 (6)
N2	0.43770 (8)	0.4859 (7)	0.3659 (2)	0.0497 (8)
N3	0.49824 (8)	0.4702 (6)	0.3018 (2)	0.0345 (5)
O1	0.26382 (8)	0.0139 (6)	0.1165 (3)	0.0724 (8)
O2	0.28892 (9)	0.1106 (6)	−0.0466 (3)	0.0679 (7)
O3	0.65877 (9)	1.1836 (7)	0.0219 (3)	0.0767 (10)
O4	0.67098 (7)	1.3101 (5)	0.1933 (3)	0.0648 (7)
Br1	0.479859 (9)	1.16298 (6)	0.04187 (3)	0.04923 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0373 (15)	0.0360 (17)	0.0391 (17)	−0.0023 (11)	0.0009 (12)	0.0032 (13)
C2	0.0461 (17)	0.051 (2)	0.0381 (17)	−0.0054 (13)	−0.0026 (13)	0.0080 (14)
C3	0.0408 (15)	0.0435 (19)	0.060 (2)	0.0051 (13)	−0.0021 (15)	−0.0033 (15)
C4	0.0349 (14)	0.0423 (18)	0.0550 (19)	0.0042 (11)	−0.0035 (14)	−0.0035 (15)
C5	0.0490 (18)	0.073 (3)	0.0444 (19)	−0.0087 (16)	0.0028 (15)	−0.0006 (17)
C6	0.0504 (18)	0.080 (3)	0.050 (2)	−0.0217 (17)	0.0059 (16)	0.0001 (18)
C7	0.0335 (14)	0.049 (2)	0.0527 (19)	0.0010 (12)	0.0005 (13)	−0.0019 (15)
C8	0.0473 (15)	0.070 (2)	0.0442 (15)	−0.0054 (13)	0.006 (2)	−0.003 (2)
C9	0.0431 (16)	0.066 (2)	0.0507 (18)	−0.0115 (15)	0.0083 (14)	0.0001 (16)

C10	0.0411 (14)	0.0516 (18)	0.063 (3)	0.0008 (13)	−0.0052 (17)	−0.0019 (19)
C11	0.083 (3)	0.087 (3)	0.072 (3)	−0.020 (2)	−0.022 (3)	−0.009 (3)
C12	0.0394 (16)	0.0411 (18)	0.056 (2)	0.0024 (13)	−0.0035 (16)	0.0029 (15)
C13	0.0333 (14)	0.0384 (17)	0.0450 (18)	0.0048 (12)	−0.0016 (13)	0.0034 (15)
C14	0.0405 (15)	0.0466 (17)	0.0392 (16)	0.0031 (12)	−0.0009 (13)	0.0001 (14)
C15	0.0393 (15)	0.0486 (19)	0.0483 (18)	−0.0006 (12)	−0.0026 (13)	−0.0061 (15)
C16	0.0367 (14)	0.0421 (18)	0.0494 (17)	0.0055 (12)	0.0017 (13)	0.0057 (14)
C17	0.0513 (18)	0.066 (3)	0.0386 (16)	−0.0032 (16)	−0.0007 (15)	0.0064 (16)
C18	0.0474 (17)	0.055 (2)	0.0405 (17)	−0.0066 (13)	−0.0061 (14)	−0.0029 (15)
C19	0.0439 (17)	0.051 (2)	0.068 (3)	0.0036 (14)	0.0061 (18)	0.0162 (19)
C20	0.0489 (19)	0.049 (2)	0.137 (4)	−0.0081 (16)	0.016 (2)	0.009 (2)
N1	0.0370 (12)	0.0420 (16)	0.0402 (14)	−0.0050 (10)	−0.0018 (12)	−0.0007 (11)
N2	0.0437 (14)	0.064 (2)	0.0408 (16)	−0.0075 (13)	0.0009 (12)	0.0105 (14)
N3	0.0365 (11)	0.0365 (14)	0.0304 (12)	−0.0044 (9)	0.0003 (9)	0.0020 (11)
O1	0.0623 (16)	0.082 (2)	0.0729 (19)	−0.0267 (15)	0.0071 (14)	−0.0048 (16)
O2	0.0654 (16)	0.0780 (19)	0.0603 (16)	−0.0199 (14)	−0.0075 (14)	−0.0071 (15)
O3	0.0720 (17)	0.087 (2)	0.071 (3)	−0.0134 (14)	0.0174 (17)	0.0213 (16)
O4	0.0499 (13)	0.0555 (16)	0.089 (2)	−0.0115 (10)	0.0067 (14)	0.0025 (15)
Br1	0.06480 (19)	0.04233 (17)	0.04057 (16)	−0.00337 (13)	−0.0031 (2)	0.0041 (2)

Geometric parameters (Å, º)

C1—N1	1.316 (4)	C11—H11B	0.9800
C1—N3	1.335 (4)	C11—H11C	0.9800
C1—H1	0.9500	C12—N3	1.486 (5)
C2—N2	1.296 (4)	C12—C13	1.522 (5)
C2—N3	1.345 (4)	C12—H12A	0.9900
C2—H2	0.9500	C12—H12B	0.9900
C3—N1	1.479 (4)	C13—C18	1.381 (5)
C3—C4	1.512 (4)	C13—C14	1.381 (5)
C3—H3A	0.9900	C14—C15	1.387 (5)
C3—H3B	0.9900	C14—H14	0.9500
C4—C5	1.382 (5)	C15—C16	1.394 (5)
C4—C9	1.383 (5)	C15—H15	0.9500
C5—C6	1.376 (5)	C16—C17	1.376 (5)
C5—H5	0.9500	C16—C19	1.482 (5)
C6—C7	1.382 (5)	C17—C18	1.388 (5)
C6—H6	0.9500	C17—H17	0.9500
C7—C8	1.388 (5)	C18—H18	0.9500
C7—C10	1.497 (5)	C19—O3	1.212 (6)
C8—C9	1.386 (5)	C19—O4	1.331 (5)
C8—H8	0.9500	C20—O4	1.449 (4)
C9—H9	0.9500	C20—H20A	0.9800
C10—O1	1.200 (5)	C20—H20B	0.9800
C10—O2	1.331 (6)	C20—H20C	0.9800
C11—O2	1.445 (5)	N1—N2	1.359 (4)
C11—H11A	0.9800		

N1—C1—N3	105.8 (3)	C13—C12—H12A	109.0
N1—C1—H1	127.1	N3—C12—H12B	109.0
N3—C1—H1	127.1	C13—C12—H12B	109.0
N2—C2—N3	111.9 (3)	H12A—C12—H12B	107.8
N2—C2—H2	124.1	C18—C13—C14	119.9 (3)
N3—C2—H2	124.1	C18—C13—C12	119.1 (3)
N1—C3—C4	110.8 (3)	C14—C13—C12	120.9 (3)
N1—C3—H3A	109.5	C13—C14—C15	120.1 (3)
C4—C3—H3A	109.5	C13—C14—H14	120.0
N1—C3—H3B	109.5	C15—C14—H14	120.0
C4—C3—H3B	109.5	C14—C15—C16	120.3 (3)
H3A—C3—H3B	108.1	C14—C15—H15	119.9
C5—C4—C9	119.3 (3)	C16—C15—H15	119.9
C5—C4—C3	120.4 (3)	C17—C16—C15	119.0 (3)
C9—C4—C3	120.3 (3)	C17—C16—C19	118.9 (3)
C6—C5—C4	120.2 (3)	C15—C16—C19	122.0 (3)
C6—C5—H5	119.9	C16—C17—C18	120.9 (3)
C4—C5—H5	119.9	C16—C17—H17	119.5
C5—C6—C7	120.9 (3)	C18—C17—H17	119.5
C5—C6—H6	119.6	C13—C18—C17	119.8 (3)
C7—C6—H6	119.6	C13—C18—H18	120.1
C6—C7—C8	119.3 (3)	C17—C18—H18	120.1
C6—C7—C10	118.4 (3)	O3—C19—O4	123.2 (4)
C8—C7—C10	122.3 (3)	O3—C19—C16	123.8 (4)
C9—C8—C7	119.7 (4)	O4—C19—C16	113.0 (3)
C9—C8—H8	120.2	O4—C20—H20A	109.5
C7—C8—H8	120.2	O4—C20—H20B	109.5
C4—C9—C8	120.7 (3)	H20A—C20—H20B	109.5
C4—C9—H9	119.6	O4—C20—H20C	109.5
C8—C9—H9	119.6	H20A—C20—H20C	109.5
O1—C10—O2	123.6 (4)	H20B—C20—H20C	109.5
O1—C10—C7	123.4 (4)	C1—N1—N2	112.0 (3)
O2—C10—C7	113.0 (3)	C1—N1—C3	127.9 (3)
O2—C11—H11A	109.5	N2—N1—C3	120.1 (3)
O2—C11—H11B	109.5	C2—N2—N1	103.4 (3)
H11A—C11—H11B	109.5	C1—N3—C2	106.9 (3)
O2—C11—H11C	109.5	C1—N3—C12	128.6 (3)
H11A—C11—H11C	109.5	C2—N3—C12	124.2 (3)
H11B—C11—H11C	109.5	C10—O2—C11	115.8 (4)
N3—C12—C13	112.9 (3)	C19—O4—C20	117.5 (4)
N3—C12—H12A	109.0		

N1—C3—C4—C5	84.0 (4)	C14—C13—C18—C17	−1.3 (5)
N1—C3—C4—C9	−95.3 (4)	C12—C13—C18—C17	−177.5 (3)
C9—C4—C5—C6	2.0 (6)	C16—C17—C18—C13	1.3 (5)
C3—C4—C5—C6	−177.3 (3)	C17—C16—C19—O3	−1.9 (6)
C4—C5—C6—C7	−1.8 (6)	C15—C16—C19—O3	175.5 (4)
C5—C6—C7—C8	0.2 (6)	C17—C16—C19—O4	177.8 (3)

C5—C6—C7—C10	179.1 (3)	C15—C16—C19—O4	−4.9 (5)
C6—C7—C8—C9	1.2 (5)	N3—C1—N1—N2	−1.9 (4)
C10—C7—C8—C9	−177.6 (3)	N3—C1—N1—C3	179.8 (3)
C5—C4—C9—C8	−0.6 (6)	C4—C3—N1—C1	111.4 (4)
C3—C4—C9—C8	178.7 (3)	C4—C3—N1—N2	−66.8 (4)
C7—C8—C9—C4	−1.0 (5)	N3—C2—N2—N1	−0.8 (4)
C6—C7—C10—O1	0.6 (5)	C1—N1—N2—C2	1.7 (4)
C8—C7—C10—O1	179.4 (3)	C3—N1—N2—C2	−179.8 (3)
C6—C7—C10—O2	−180.0 (4)	N1—C1—N3—C2	1.3 (4)
C8—C7—C10—O2	−1.1 (5)	N1—C1—N3—C12	175.9 (3)
N3—C12—C13—C18	−90.6 (4)	N2—C2—N3—C1	−0.3 (4)
N3—C12—C13—C14	93.2 (4)	N2—C2—N3—C12	−175.2 (3)
C18—C13—C14—C15	0.1 (5)	C13—C12—N3—C1	35.4 (5)
C12—C13—C14—C15	176.2 (3)	C13—C12—N3—C2	−150.9 (3)
C13—C14—C15—C16	1.1 (5)	O1—C10—O2—C11	−1.6 (6)
C14—C15—C16—C17	−1.1 (5)	C7—C10—O2—C11	178.9 (3)
C14—C15—C16—C19	−178.4 (3)	O3—C19—O4—C20	−0.9 (5)
C15—C16—C17—C18	−0.1 (5)	C16—C19—O4—C20	179.4 (3)
C19—C16—C17—C18	177.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···Br1	0.95	2.61	3.461 (3)	149
C3—H3*A*···Br1	0.99	2.91	3.795 (4)	149
C2—H2···Br1^{i}	0.95	2.75	3.657 (3)	161

Symmetry code: (i) −*x*+1, −*y*+1, *z*+1/2.