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4-Bromo-*N*-(2-nitrophenyl)benzamide

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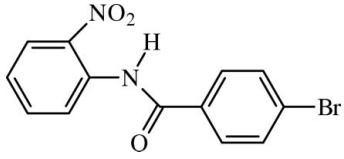
Key indicators: single-crystal X-ray study; T = 123 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.135; data-to-parameter ratio = 29.0.

The title nitrophenyl benzamide, $C_{13}H_9BrN_2O_3$, with two molecules in the asymmetric unit, has dihedral angles of 16.78 (15) and 18.87 (14)° between the benzene rings. An intramolecular N—H···O hydrogen bond is observed in each molecule. In the crystal, the molecules are linked by weak C—H···O interactions; halogen–halogen interactions are also observed [Br···Br = 3.4976 (7) Å]. These interactions form $R_2^2(10)$, $R_2^2(15)$ and $R_6^6(32)$ edge-fused rings along [010].

Related literature

For properties of amide compounds, see: Bisson *et al.* (2000). For the antibacterial and antifungal activity of amide compounds, see: Aytemir *et al.* (2003). For similar compounds, see: Moreno-Fuquen *et al.* (2013); Sripet *et al.* (2012). For halogen–halogen interactions, see: Awwadi *et al.* (2006); For hydrogen-bonding information, see: Nardelli (1995). For hydrogen-bond motifs, see: Etter (1990).



Experimental

Crystal data

$C_{13}H_9BrN_2O_3$
M_r = 321.13
Triclinic, $P\overline{1}$
a = 3.8338 (4) Å
b = 12.6784 (13) Å
c = 24.918 (2) Å
α = 81.875 (8)°
β = 88.386 (7)°
γ = 85.460 (8)°
V = 1195.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.45 mm^{-1}
T = 123 K
0.49 × 0.05 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2010; analytical numeric absorption correction using a multi-faceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.380, T_{max} = 0.914
9979 measured reflections
9979 independent reflections
7814 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
S = 1.04
9979 reflections
344 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O4^{i}	0.95	2.65	3.378 (5)	134
C16—H16···O2^{ii}	0.95	2.64	3.349 (5)	132
C19—H19···O1^{iii}	0.95	2.52	3.262 (5)	135
C3—H3···O5^{iv}	0.95	2.58	3.299 (5)	133
C23—H23···O6^{v}	0.95	2.56	3.334 (5)	139
N1—H1*N*···O2	0.88	1.92	2.615 (5)	134
N3—H3*N*···O5	0.88	1.92	2.628 (5)	136

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $x, y-1, z$; (iv) $x, y+1, z$; (v) $-x-1, -y, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); 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: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: GG2134).

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supporting information

Acta Cryst. (2014). E**70**, o344 [doi:10.1107/S1600536814003298]

4-Bromo-*N*-(2-nitrophenyl)benzamide

Rodolfo Moreno-Fuquen, Alexis Azcárate and Alan R. Kennedy

S1. Experimental

S1.1. Synthesis and crystallization

The reagents and solvents for the synthesis were obtained from the Aldrich Chemical Co., and were used without additional purification. The title molecule was synthesized using equimolar quantities of 4-bromobenzoyl chloride (0.328 g., 1.495 mmol) and 2-nitroaniline (0.206 g). The reagents were dissolved in 10 mL of acetonitrile and the solution was taken to reflux in constant stirring for 1 hour. Yellow crystals of good quality were obtained after leaving the solvent to evaporate. Yellow crystals of good quality were obtained with m.p of 423 (1)K.

S1.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H-atoms were positioned at geometrically idealized positions with C—H distance of 0.95 Å and N—H distance of 0.88 Å and U_{iso}(H) = 1.2 times U_{eq} of the atoms to which they were bonded.

S2. Results and discussion

The present compound forms part of a systematic work on N-aromatic amides. The formation of oligomers with properties of molecular zippers have been obtained using molecular templates which include amido ligands (Bisson *et al.*, 2000). Antibacterial and antifungal activities of different carboxyamide derivatives have been reported (Aytemir *et al.*, 2003). In the synthesis of amides in our group, the 2-nitroaniline is taken as a template, in order to study the structural changes and the supramolecular behavior by the reaction of different ligands with this precursor (Moreno-Fuquen *et al.*, 2013). In the reactions involving the 2-nitroaniline, as precursor, we aimed to synthesize the N-(2-nitrophenyl)-4-bromo-benzamide (I). A close structure, the 4-bromo-N-(4-methoxy-2-nitrophenyl)-benzamide, (4MNB), (Sripet *et al.*, 2012), has been used as comparison with the structural parameters of the title compound. The title compound has two molecules (A and B) per asymmetric unit (see Fig. 1). The compound exhibits dihedral angles between the benzene rings, very similar: 16.78 (15)° and 18.87 (14)° for A and B molecules, respectively. These dihedral angles are somewhat different when compared with the related compound (4MNB) [2.90 (8)°]. In (I) the other bond lengths and bond angles agree closely with those values presented in its homologous amide (4MNB). The nitro groups form dihedral angles with the adjacent benzene ring of 6.7 (2)° and 9.9 (2)° for O2—N2—O3 and O5—N4—O6, respectively. The crystal packing shows no classical intermolecular hydrogen bonds and the molecules pack by forming weak C—H···O interactions that are propagated along [010] (see Fig. 2). According to the graph-set assignment, the intramolecular hydrogen-bond pattern generates a S(6) ring motif (Etter, 1990). The crystal packing is stabilized by weak C—H···O intermolecular interactions. The C6 and C3 atoms of the phenyl ring at (x,y,z) act as hydrogen-bond donors to carbonyl O4 atom at (x-1, +y, +z) and to nitro O5 atom at (x,+y+1,+z) respectively. The C16 and C19 atoms of the phenyl ring at (x, y, z) act as hydrogen-bond donors to nitro O2 atom at (x+1, y, z) and to carbonyl O1 atom at (x,y-1,z), respectively. Additionally the C23 atom at

(x,y,z) acts as a hydrogen-bond donor to nitro O6 atom at (-x-1, -y, -z+1), (see Table 1; Nardelli, 1995). All these interactions form $R^2_2(10)$, $R^2_2(15)$ and $R^6_6(32)$ edge-fused rings along the [010] direction (see Fig. 2). Recent theoretical calculations show that halogen···halogen interactions are controlled by electrostatic forces and they display directional character (Awwadi *et al.*, 2006). In the title structure, halogen···halogen interactions [Br···Br = 3.4976 (7) Å] within the chains stabilized by C—H···O interactions are observed. This Br···Br distance is much shorter than the sum of the van der Waals radii (3.70 Å).

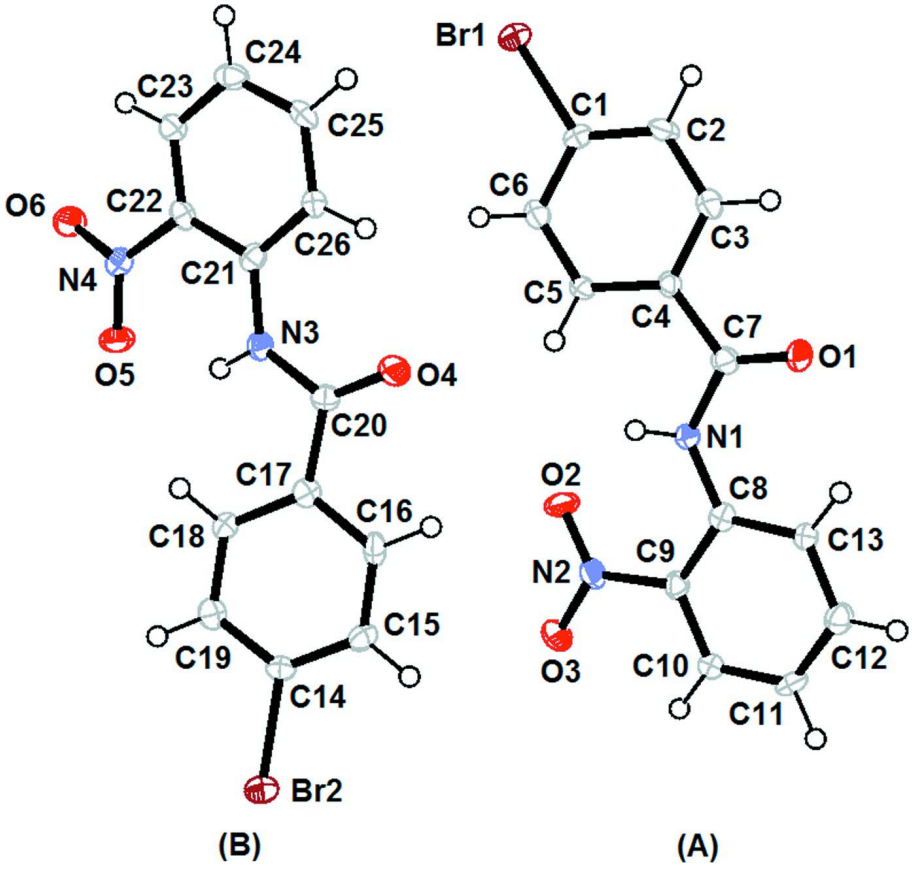

Figure 1

Molecular conformation and atom numbering scheme for the title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

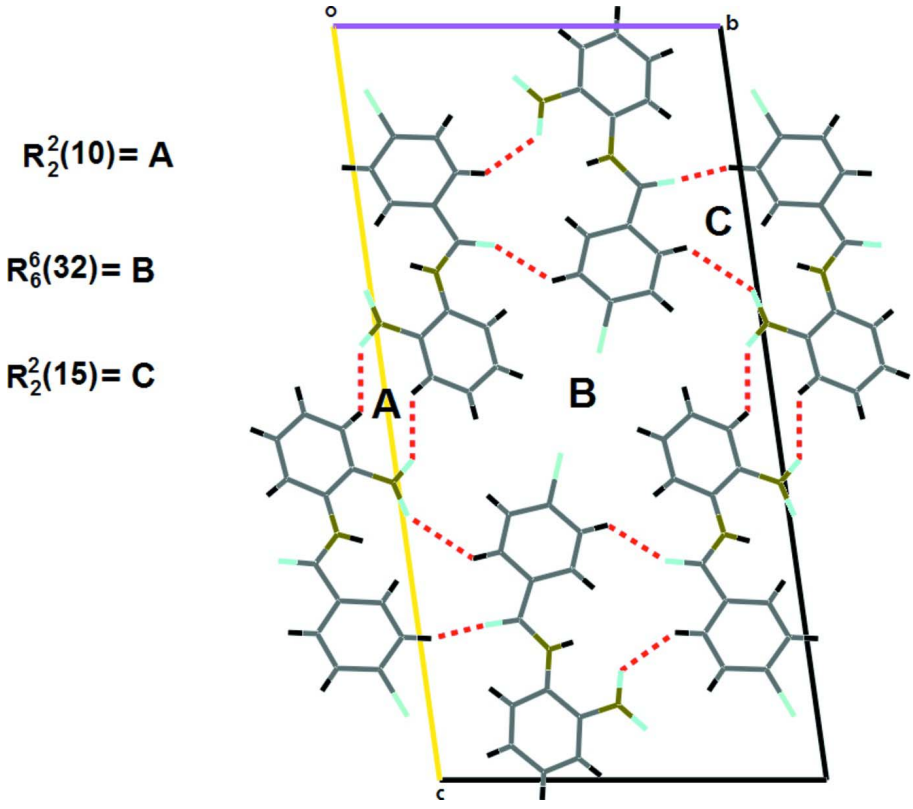

Figure 2

Part of the crystal structure of (I), showing the formation of edge-fused $R^2_2(10)$, $R^2_2(15)$ and $R^2_2(32)$ rings running along [010].

4-Bromo-*N*-(2-nitrophenyl)-benzamide

Crystal data

$C_{13}H_9BrN_2O_3$
M_r = 321.13
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 3.8338 (4) Å
b = 12.6784 (13) Å
c = 24.918 (2) Å
α = 81.875 (8)°
β = 88.386 (7)°
γ = 85.460 (8)°
V = 1195.1 (2) Å^3
Z = 4
F(000) = 640
D_x = 1.785 Mg m^{-3}
Melting point: 423(1) K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4010 reflections
θ = 3.1–28.0°
μ = 3.45 mm^{-1}
T = 123 K
Needle, yellow
0.49 × 0.05 × 0.03 mm

Data collection

Oxford Diffraction Xcalibur E diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: analytical [*CrysAlis PRO* (Oxford Diffraction, 2010; analytical numeric absorption correction using a multi-faceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.380, T_{max} = 0.914
9979 measured reflections
9979 independent reflections

7814 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 27.0°$, $\theta_{min} = 3.2°$
$h = -4 \rightarrow 4$
$k = -14 \rightarrow 16$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.135$
$S = 1.04$
9979 reflections
344 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
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 3.1562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Br1	−0.49930 (10)	0.56740 (4)	0.433729 (18)	0.02208 (13)
Br2	0.96920 (10)	0.05996 (4)	0.084392 (18)	0.02296 (13)
O1	0.2537 (8)	0.8253 (2)	0.20551 (12)	0.0270 (7)
O2	−0.0265 (8)	0.4919 (3)	0.14483 (13)	0.0334 (8)
O3	0.1224 (9)	0.4476 (3)	0.06706 (14)	0.0384 (9)
O4	0.4069 (8)	0.3367 (3)	0.29067 (13)	0.0313 (8)
O5	−0.0468 (8)	−0.0126 (2)	0.35060 (13)	0.0312 (8)
O6	−0.3517 (8)	−0.0460 (2)	0.42413 (13)	0.0285 (8)
N1	0.1677 (9)	0.6691 (3)	0.17304 (14)	0.0202 (8)
H1N	0.0934	0.6052	0.1830	0.024*
N2	0.1123 (9)	0.5117 (3)	0.09994 (16)	0.0229 (9)
N3	0.2077 (8)	0.1750 (3)	0.32592 (14)	0.0197 (8)
H3N	0.1732	0.1120	0.3170	0.024*
N4	−0.1642 (9)	0.0120 (3)	0.39439 (15)	0.0209 (8)
C1	−0.3041 (10)	0.6174 (3)	0.36484 (17)	0.0168 (9)
C2	−0.2476 (11)	0.7244 (3)	0.35235 (18)	0.0214 (10)
H2	−0.3098	0.7727	0.3775	0.026*
C3	−0.0988 (10)	0.7599 (4)	0.30253 (18)	0.0215 (10)
H3	−0.0561	0.8331	0.2937	0.026*
C4	−0.0101 (10)	0.6895 (3)	0.26489 (17)	0.0158 (9)
C5	−0.0678 (10)	0.5813 (3)	0.27900 (17)	0.0180 (9)
H5	−0.0041	0.5321	0.2543	0.022*

C6	−0.2171 (10)	0.5459 (3)	0.32875 (17)	0.0201 (10)
H6	−0.2598	0.4728	0.3381	0.024*
C7	0.1510 (10)	0.7357 (3)	0.21253 (18)	0.0194 (10)
C8	0.2861 (10)	0.6897 (3)	0.11986 (17)	0.0173 (9)
C9	0.2622 (10)	0.6145 (3)	0.08342 (18)	0.0186 (9)
C10	0.3722 (10)	0.6340 (3)	0.02913 (17)	0.0194 (10)
H10	0.3486	0.5824	0.0056	0.023*
C11	0.5139 (10)	0.7282 (3)	0.01035 (18)	0.0212 (10)
H11	0.5915	0.7424	−0.0263	0.025*
C12	0.5432 (10)	0.8028 (4)	0.04532 (18)	0.0228 (10)
H12	0.6411	0.8682	0.0321	0.027*
C13	0.4345 (10)	0.7847 (3)	0.09874 (18)	0.0193 (10)
H13	0.4604	0.8375	0.1216	0.023*
C14	0.7748 (10)	0.1158 (3)	0.14657 (17)	0.0177 (9)
C15	0.7605 (10)	0.2246 (3)	0.14817 (18)	0.0200 (10)
H15	0.8432	0.2718	0.1183	0.024*
C16	0.6236 (10)	0.2633 (3)	0.19396 (18)	0.0213 (10)
H16	0.6128	0.3378	0.1957	0.026*
C17	0.5013 (10)	0.1945 (3)	0.23763 (17)	0.0184 (10)
C18	0.5160 (10)	0.0848 (3)	0.23493 (18)	0.0193 (10)
H18	0.4291	0.0375	0.2644	0.023*
C19	0.6571 (10)	0.0450 (4)	0.18936 (18)	0.0202 (10)
H19	0.6726	−0.0296	0.1875	0.024*
C20	0.3678 (11)	0.2434 (4)	0.28646 (18)	0.0194 (10)
C21	0.0933 (10)	0.1912 (3)	0.37755 (17)	0.0180 (9)
C22	−0.0783 (10)	0.1120 (3)	0.41268 (18)	0.0187 (10)
C23	−0.1763 (10)	0.1250 (3)	0.46513 (18)	0.0204 (10)
H23	−0.2880	0.0701	0.4875	0.024*
C24	−0.1133 (11)	0.2167 (4)	0.48520 (18)	0.0233 (10)
H24	−0.1778	0.2254	0.5215	0.028*
C25	0.0461 (10)	0.2968 (3)	0.45179 (18)	0.0198 (10)
H25	0.0882	0.3608	0.4654	0.024*
C26	0.1440 (10)	0.2850 (3)	0.39935 (18)	0.0197 (10)
H26	0.2486	0.3418	0.3773	0.024*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0215 (2)	0.0273 (3)	0.0174 (3)	−0.00393 (18)	0.00245 (17)	−0.00226 (19)
Br2	0.0207 (2)	0.0277 (3)	0.0208 (3)	−0.00279 (18)	0.00324 (17)	−0.0047 (2)
O1	0.0428 (19)	0.0170 (18)	0.0223 (19)	−0.0113 (14)	0.0046 (15)	−0.0028 (14)
O2	0.052 (2)	0.031 (2)	0.020 (2)	−0.0187 (16)	0.0162 (16)	−0.0100 (15)
O3	0.067 (2)	0.020 (2)	0.032 (2)	−0.0136 (17)	0.0130 (18)	−0.0141 (16)
O4	0.047 (2)	0.021 (2)	0.028 (2)	−0.0090 (15)	0.0118 (15)	−0.0079 (15)
O5	0.049 (2)	0.027 (2)	0.020 (2)	−0.0157 (15)	0.0125 (15)	−0.0091 (15)
O6	0.0359 (18)	0.0234 (19)	0.028 (2)	−0.0123 (14)	0.0114 (15)	−0.0056 (15)
N1	0.029 (2)	0.014 (2)	0.018 (2)	−0.0049 (15)	0.0032 (16)	−0.0033 (15)
N2	0.029 (2)	0.016 (2)	0.024 (2)	−0.0024 (16)	−0.0005 (17)	−0.0049 (17)

N3	0.0251 (19)	0.014 (2)	0.020 (2)	−0.0045 (15)	0.0007 (15)	−0.0029 (16)
N4	0.0220 (19)	0.021 (2)	0.019 (2)	−0.0017 (15)	−0.0012 (16)	0.0000 (17)
C1	0.014 (2)	0.022 (3)	0.014 (2)	−0.0017 (17)	0.0008 (16)	−0.0008 (18)
C2	0.024 (2)	0.023 (3)	0.019 (3)	−0.0006 (19)	0.0036 (18)	−0.010 (2)
C3	0.025 (2)	0.017 (2)	0.024 (3)	−0.0035 (18)	−0.0004 (19)	−0.0044 (19)
C4	0.018 (2)	0.013 (2)	0.016 (2)	−0.0002 (16)	−0.0023 (17)	−0.0016 (17)
C5	0.024 (2)	0.016 (2)	0.016 (2)	−0.0044 (17)	0.0020 (18)	−0.0056 (18)
C6	0.022 (2)	0.016 (2)	0.022 (3)	−0.0012 (17)	−0.0036 (18)	−0.0041 (19)
C7	0.019 (2)	0.019 (3)	0.019 (3)	0.0025 (18)	−0.0001 (17)	−0.0024 (19)
C8	0.013 (2)	0.019 (2)	0.019 (3)	−0.0009 (16)	−0.0022 (17)	−0.0006 (18)
C9	0.020 (2)	0.015 (2)	0.021 (3)	−0.0043 (17)	0.0003 (18)	−0.0019 (18)
C10	0.022 (2)	0.017 (2)	0.019 (3)	−0.0009 (17)	0.0042 (18)	−0.0031 (18)
C11	0.021 (2)	0.029 (3)	0.012 (2)	−0.0021 (18)	0.0040 (17)	0.0013 (19)
C12	0.021 (2)	0.022 (3)	0.025 (3)	−0.0058 (18)	0.0020 (19)	−0.001 (2)
C13	0.023 (2)	0.015 (2)	0.019 (3)	−0.0040 (17)	0.0042 (18)	−0.0027 (18)
C14	0.015 (2)	0.021 (3)	0.017 (2)	−0.0007 (17)	0.0004 (17)	−0.0050 (18)
C15	0.019 (2)	0.023 (3)	0.017 (3)	−0.0059 (18)	0.0026 (18)	−0.0010 (19)
C16	0.021 (2)	0.012 (2)	0.029 (3)	−0.0024 (17)	−0.0003 (19)	0.0019 (19)
C17	0.016 (2)	0.020 (3)	0.020 (3)	−0.0047 (17)	−0.0015 (17)	−0.0037 (19)
C18	0.021 (2)	0.018 (2)	0.018 (3)	−0.0022 (17)	0.0030 (18)	−0.0002 (19)
C19	0.018 (2)	0.019 (3)	0.024 (3)	−0.0033 (17)	−0.0022 (18)	−0.0030 (19)
C20	0.022 (2)	0.020 (3)	0.017 (3)	−0.0017 (18)	−0.0008 (18)	−0.0041 (19)
C21	0.015 (2)	0.020 (3)	0.018 (2)	0.0002 (17)	−0.0015 (17)	0.0011 (18)
C22	0.016 (2)	0.016 (2)	0.025 (3)	0.0016 (16)	−0.0027 (18)	−0.0042 (19)
C23	0.022 (2)	0.019 (3)	0.020 (3)	0.0008 (18)	0.0001 (18)	−0.0035 (19)
C24	0.021 (2)	0.030 (3)	0.018 (3)	0.0067 (19)	−0.0013 (18)	−0.006 (2)
C25	0.020 (2)	0.017 (2)	0.024 (3)	0.0017 (17)	−0.0022 (18)	−0.0094 (19)
C26	0.024 (2)	0.015 (2)	0.020 (3)	−0.0010 (17)	0.0020 (18)	−0.0014 (18)

Geometric parameters (Å, º)

Br1—C1	1.898 (4)	C9—C10	1.400 (6)
Br2—C14	1.902 (4)	C10—C11	1.368 (6)
O1—C7	1.219 (5)	C10—H10	0.9500
O2—N2	1.227 (5)	C11—C12	1.386 (6)
O3—N2	1.230 (5)	C11—H11	0.9500
O4—C20	1.223 (5)	C12—C13	1.377 (6)
O5—N4	1.239 (5)	C12—H12	0.9500
O6—N4	1.227 (4)	C13—H13	0.9500
N1—C7	1.382 (5)	C14—C15	1.383 (6)
N1—C8	1.385 (5)	C14—C19	1.383 (6)
N1—H1N	0.8800	C15—C16	1.378 (6)
N2—C9	1.467 (5)	C15—H15	0.9500
N3—C20	1.380 (5)	C16—C17	1.390 (6)
N3—C21	1.385 (5)	C16—H16	0.9500
N3—H3N	0.8800	C17—C18	1.399 (6)
N4—C22	1.470 (5)	C17—C20	1.502 (6)
C1—C6	1.381 (6)	C18—C19	1.386 (6)

C1—C2	1.382 (6)	C18—H18	0.9500
C2—C3	1.383 (6)	C19—H19	0.9500
C2—H2	0.9500	C21—C26	1.404 (6)
C3—C4	1.401 (6)	C21—C22	1.425 (6)
C3—H3	0.9500	C22—C23	1.378 (6)
C4—C5	1.400 (6)	C23—C24	1.370 (6)
C4—C7	1.491 (6)	C23—H23	0.9500
C5—C6	1.382 (6)	C24—C25	1.388 (6)
C5—H5	0.9500	C24—H24	0.9500
C6—H6	0.9500	C25—C26	1.374 (6)
C8—C13	1.402 (6)	C25—H25	0.9500
C8—C9	1.415 (6)	C26—H26	0.9500

C7—N1—C8	128.5 (4)	C13—C12—C11	121.9 (4)
C7—N1—H1N	115.8	C13—C12—H12	119.1
C8—N1—H1N	115.8	C11—C12—H12	119.1
O2—N2—O3	121.3 (4)	C12—C13—C8	120.9 (4)
O2—N2—C9	120.5 (4)	C12—C13—H13	119.5
O3—N2—C9	118.1 (4)	C8—C13—H13	119.5
C20—N3—C21	129.4 (4)	C15—C14—C19	122.1 (4)
C20—N3—H3N	115.3	C15—C14—Br2	119.6 (3)
C21—N3—H3N	115.3	C19—C14—Br2	118.3 (3)
O6—N4—O5	121.7 (4)	C16—C15—C14	118.6 (4)
O6—N4—C22	117.7 (4)	C16—C15—H15	120.7
O5—N4—C22	120.6 (4)	C14—C15—H15	120.7
C6—C1—C2	121.5 (4)	C15—C16—C17	120.8 (4)
C6—C1—Br1	119.4 (3)	C15—C16—H16	119.6
C2—C1—Br1	119.0 (3)	C17—C16—H16	119.6
C1—C2—C3	118.7 (4)	C16—C17—C18	119.5 (4)
C1—C2—H2	120.6	C16—C17—C20	117.1 (4)
C3—C2—H2	120.6	C18—C17—C20	123.4 (4)
C2—C3—C4	121.0 (4)	C19—C18—C17	120.1 (4)
C2—C3—H3	119.5	C19—C18—H18	120.0
C4—C3—H3	119.5	C17—C18—H18	120.0
C5—C4—C3	118.8 (4)	C14—C19—C18	118.8 (4)
C5—C4—C7	124.4 (4)	C14—C19—H19	120.6
C3—C4—C7	116.7 (4)	C18—C19—H19	120.6
C6—C5—C4	120.1 (4)	O4—C20—N3	123.4 (4)
C6—C5—H5	119.9	O4—C20—C17	121.5 (4)
C4—C5—H5	119.9	N3—C20—C17	115.1 (4)
C1—C6—C5	119.7 (4)	N3—C21—C26	122.7 (4)
C1—C6—H6	120.1	N3—C21—C22	121.8 (4)
C5—C6—H6	120.1	C26—C21—C22	115.4 (4)
O1—C7—N1	123.6 (4)	C23—C22—C21	122.3 (4)
O1—C7—C4	122.3 (4)	C23—C22—N4	116.4 (4)
N1—C7—C4	114.2 (4)	C21—C22—N4	121.4 (4)
N1—C8—C13	122.8 (4)	C24—C23—C22	120.3 (4)
N1—C8—C9	121.2 (4)	C24—C23—H23	119.8

C13—C8—C9	116.0 (4)	C22—C23—H23	119.8
C10—C9—C8	122.5 (4)	C23—C24—C25	119.1 (4)
C10—C9—N2	115.5 (4)	C23—C24—H24	120.4
C8—C9—N2	122.0 (4)	C25—C24—H24	120.4
C11—C10—C9	119.3 (4)	C26—C25—C24	121.2 (4)
C11—C10—H10	120.4	C26—C25—H25	119.4
C9—C10—H10	120.4	C24—C25—H25	119.4
C10—C11—C12	119.4 (4)	C25—C26—C21	121.7 (4)
C10—C11—H11	120.3	C25—C26—H26	119.2
C12—C11—H11	120.3	C21—C26—H26	119.2

O2—O2—N2—O3	0.0 (3)	N1—C8—C13—C12	−178.8 (3)
O2—O2—N2—C9	0.0 (4)	C9—C8—C13—C12	1.0 (5)
O5—O5—N4—O6	0.0 (12)	C19—C14—C15—C16	−0.1 (6)
O5—O5—N4—C22	0.0 (13)	Br2—C14—C15—C16	−179.0 (3)
C6—C1—C2—C3	−0.3 (6)	C14—C15—C16—C17	−0.2 (6)
Br1—C1—C2—C3	178.7 (3)	C15—C16—C17—C18	−0.3 (6)
C1—C2—C3—C4	0.8 (6)	C15—C16—C17—C20	178.0 (4)
C2—C3—C4—C5	−1.4 (6)	C16—C17—C18—C19	1.1 (6)
C2—C3—C4—C7	−179.6 (3)	C20—C17—C18—C19	−177.1 (4)
C3—C4—C5—C6	1.5 (6)	C15—C14—C19—C18	0.9 (6)
C7—C4—C5—C6	179.6 (3)	Br2—C14—C19—C18	179.8 (3)
C2—C1—C6—C5	0.4 (6)	C17—C18—C19—C14	−1.4 (5)
Br1—C1—C6—C5	−178.6 (3)	C21—N3—C20—O4	−6.5 (6)
C4—C5—C6—C1	−1.0 (6)	C21—N3—C20—C17	172.1 (3)
C8—N1—C7—O1	−2.2 (6)	C16—C17—C20—O4	−9.4 (6)
C8—N1—C7—C4	176.8 (3)	C18—C17—C20—O4	168.8 (4)
C5—C4—C7—O1	−166.6 (4)	C16—C17—C20—N3	172.0 (3)
C3—C4—C7—O1	11.5 (6)	C18—C17—C20—N3	−9.8 (5)
C5—C4—C7—N1	14.3 (5)	C20—N3—C21—C26	−3.4 (6)
C3—C4—C7—N1	−167.5 (3)	C20—N3—C21—C22	178.0 (4)
C7—N1—C8—C13	4.4 (6)	N3—C21—C22—C23	176.4 (3)
C7—N1—C8—C9	−175.5 (4)	C26—C21—C22—C23	−2.3 (5)
N1—C8—C9—C10	178.5 (3)	N3—C21—C22—N4	−4.3 (5)
C13—C8—C9—C10	−1.4 (6)	C26—C21—C22—N4	177.0 (3)
N1—C8—C9—N2	−0.1 (6)	O6—N4—C22—C23	8.7 (5)
C13—C8—C9—N2	−179.9 (3)	O5—N4—C22—C23	−170.6 (3)
O2—N2—C9—C10	−172.0 (4)	O5—N4—C22—C23	−170.6 (3)
O2—N2—C9—C10	−172.0 (4)	O6—N4—C22—C21	−170.6 (3)
O3—N2—C9—C10	6.2 (5)	O5—N4—C22—C21	10.1 (5)
O2—N2—C9—C8	6.7 (6)	O5—N4—C22—C21	10.1 (5)
O2—N2—C9—C8	6.7 (6)	C21—C22—C23—C24	0.7 (6)
O3—N2—C9—C8	−175.1 (4)	N4—C22—C23—C24	−178.6 (3)
C8—C9—C10—C11	1.1 (6)	C22—C23—C24—C25	0.8 (6)
N2—C9—C10—C11	179.8 (3)	C23—C24—C25—C26	−0.6 (6)
C9—C10—C11—C12	−0.5 (6)	C24—C25—C26—C21	−1.1 (6)
C10—C11—C12—C13	0.2 (6)	N3—C21—C26—C25	−176.2 (3)
C11—C12—C13—C8	−0.5 (6)	C22—C21—C26—C25	2.5 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O4^{i}	0.95	2.65	3.378 (5)	134
C16—H16···O2^{ii}	0.95	2.64	3.349 (5)	132
C19—H19···O1^{iii}	0.95	2.52	3.262 (5)	135
C3—H3···O5^{iv}	0.95	2.58	3.299 (5)	133
C23—H23···O6^{v}	0.95	2.56	3.334 (5)	139
N1—H1*N*···O2	0.88	1.92	2.615 (5)	134
N3—H3*N*···O5	0.88	1.92	2.628 (5)	136

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $x, y-1, z$; (iv) $x, y+1, z$; (v) $-x-1, -y, -z+1$.