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Crystal structure of *N*-(7-dibromomethyl-5-methyl-1,8-naphthyridin-2-yl)benzamide–pyrrolidine-2,5-dione (1/1)

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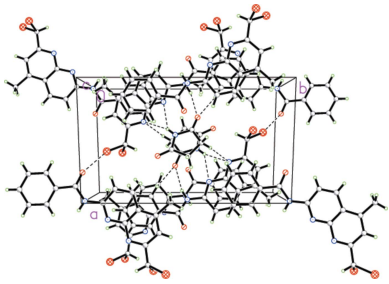
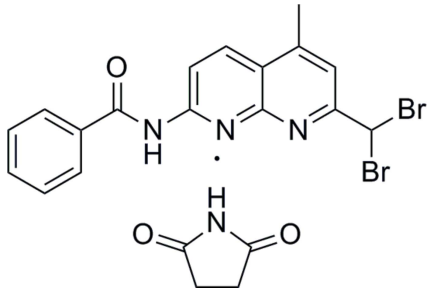
The title compound, $C_{17}H_{13}Br_2N_3O\cdot C_4H_5NO_2$, is a co-crystal of *N*-(7-dibromomethyl-5-methyl-1,8-naphthyridin-2-yl)benzamide and pyrrolidine-2,5-dione (succinimide). The benzamide molecule exhibits pseudo-mirror symmetry, with an r.m.s. deviation of the non-H atoms of 0.09 Å (except for the two Br atoms). The angle between the least-squares planes of the two molecules is 26.2 (2)°. In the crystal, the two molecules are mutually linked by N—H···O and N—H···N hydrogen bonds. The packing is consolidated by C—H···(O,N) hydrogen bonds and π–π stacking interactions.

1. Chemical context

1,8-Naphthyridine derivatives are important heterocyclic compounds that exhibit excellent biochemical and pharmacological properties. Moreover, these compounds benefit from conjugate π-electronic structures and are widely used as ligands in the synthesis of metal complexes (Tang *et al.*, 2015; Matveeva *et al.*, 2012, 2013), functional materials (Kuo *et al.*, 2011; Katz *et al.*, 2007; Hu & Chen, 2010) or as catalysts (Fuentes *et al.*, 2011; Yamazaki *et al.*, 2011). In a number of studies, the fluorescent properties of naphthyridines have been investigated (Yu *et al.*, 2013; Li *et al.*, 2012), in particular as selective fluorescent chemosensors for small biological molecules through hydrogen bonding (Nakatani *et al.*, 2013; Liang *et al.*, 2012). 1,8-Naphthyridin–BF_2 complexes are known to be fluorescent dyes with high chemical stability (Li *et al.*, 2014), high fluorescence quantum yields (Quan *et al.*, 2012), high extinction coefficients (Wu *et al.*, 2013) and sharp fluorescence peaks (Du *et al.*, 2014). Some antiviral medications are also based on 1,8-naphthyridines (Elansary *et al.*, 2014). In this context we aimed to synthesize the title 1,8-naphthyridine derivative and report here on the crystal structure of the obtained co-crystal with pyrrolidine-2,5-dione (succinimide).





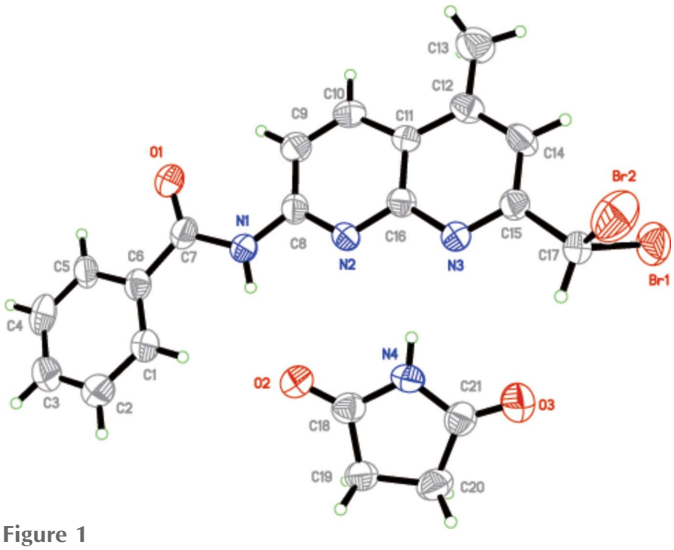


Figure 1
The molecular components in the title co-crystal, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

2. Structural commentary

The molecular structure of the title 1,8-naphthyridine derivative is shown in Fig. 1. The *N*-(7-(dibromomethyl)-5-methyl-1,8-naphthyridin-2-yl)benzamide moiety (except the two Br atoms) is essentially planar (r.m.s deviation = 0.09 Å), with the maximum deviation from the mean plane being 0.315 (5) Å for atom O1. The naphthyridine ring system makes a dihedral angle of 2.2 (2)° with the benzene ring and is oriented at an angle of 26.2 (2)° relative to the succinimide. The conformation of the C═O and the N—H bonds of the amide segment are *anti* to one another, similar to that reported for benzamide moiety in *N*-{4-[(6-chloropyridin-3-yl)-methoxy]phenyl}-2,6-difluorobenzamide (Liang *et al.*, 2016).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2	0.86	2.22	3.060 (7)	164
N4—H4*A*···N2	0.86	2.48	3.195 (7)	141
N4—H4*A*···N3	0.86	2.27	3.098 (7)	162
C1—H1*B*···O2	0.93	2.43	3.299 (8)	156
C9—H9*A*···O1	0.93	2.30	2.870 (8)	119
C17—H17*A*···O3	0.98	2.60	3.504 (8)	154
C19—H19*B*···N3^{i}	0.97	2.58	3.538 (8)	170

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

3. Supramolecular features

The two molecules are mutually linked into pairs by N—H···O and N—H···N hydrogen bonds with the (imide)N—H···N bond bifurcated (Table 1, Fig. 2). In the 1,8-naphthyridine derivative, an intramolecular C—H···O hydrogen bond between a phenyl H atom and the carbonyl function is also present. Apart from the classical hydrogen-bonding interactions, the two molecules are additionally linked by weaker C—H···O and C—H···N hydrogen bonds. These pairs are linked by weak C—Br···O interactions [3.094 (5) Å]. The supramolecular aggregation is completed by π–π stacking interactions between two neighbouring succinimide molecules with a centroid-to-centroid distance of $Cg\cdots Cg^{i}$ = 3.854 (4) Å [interplanar distance = 3.172 (3) Å; symmetry code: $-x+1, -y+1, -z+1$], forming a three-dimensional supramolecular network (Fig. 3).

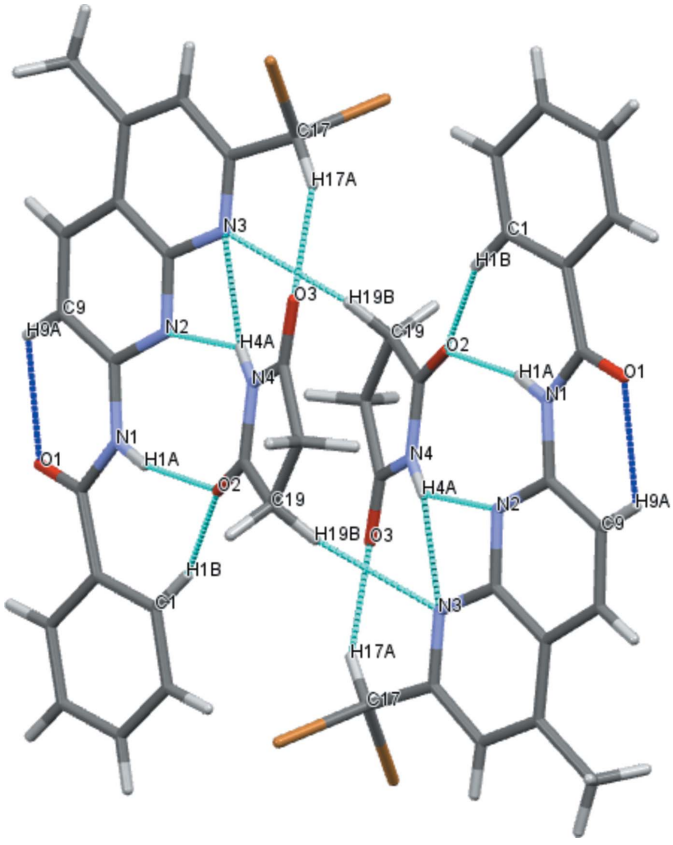


Figure 2
The different types of hydrogen bonds between the two molecules and pairs of molecules; intramolecular hydrogen bonds are shown as blue dashed lines and intermolecular hydrogen bonds are shown as turquoise dashed lines.

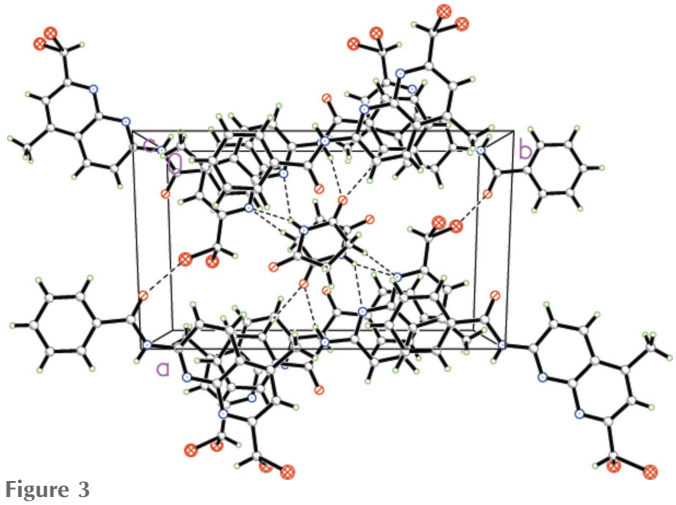


Figure 3
A view along the *c* axis, showing the crystal packing of the title compound.

4. Database survey

In the Cambridge Structural Database (Version 5.37; Groom *et al.*, 2016), the structural data for a very similar 1,8-naphthyridine derivative have been deposited (CSD refcode LESBOC; Gou *et al.*, 2013). Instead of a benzamide, the latter is an acetamide where the dihedral angle between the naphthyridine moiety and the succinimide co-molecule is 14.1°.

5. Synthesis and crystallization

N-(5,7-dimethyl-1,8-naphthyridin-2-yl)benzamide (Wu *et al.*, 2012) (0.277 g,1 mmol) and *N*-bromosuccinimide (0.356 g, 2 mmol) were added to an dry acetonitrile (30 ml) solution under nitrogen atmosphere. The mixture was refluxed at room temperature in the presence of light with a 250 W infrared lamp for 4 h. Excess solvent was removed and the crude product was purified by column chromatography using dichloromethane/methanol (120:1) as the mobile phase to give a light-yellow powder (yield: 0.1 g; 19%). Crystals suitable for X-ray analysis were obtained by slow diffusion of a dichloromethane solution at ambient temperature. Several cycles of purification by chromatography were used to reduce the amount of succinimide.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were constrained to an ideal geometry with C—H distances in the range 0.93–0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and U_{iso}(H) = 1.2U_{eq}(C) for all other H atoms, and with N—H = 0.86 Å, U_{iso}(H) = 1.2U_{eq}(N).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{13}Br_2N_3O{\cdot}C_4H_5NO_2$
M_r	534.21
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, b, c (Å)	9.6931 (19), 15.699 (3), 14.614 (3)
β (°)	108.99 (3)
V (Å^3)	2103.0 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.89
Crystal size (mm)	0.30 × 0.28 × 0.26
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR* ; Higashi, 1995)
T_{min}, T_{max}	0.389, 0.432
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16558, 4129, 2010
R_{int}	0.125
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.148, 0.98
No. of reflections	4129
No. of parameters	271
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.35, −0.43

Computer programs: *PROCESS-AUTO* (Rigaku, 1998), *CrystalStructure* (Rigaku/MSC, 2006), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999).

Acknowledgements

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supporting information

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Computing details

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

N-(7-Dibromomethyl-5-methyl-1,8-naphthyridin-2-yl)benzamide–pyrrolidine-2,5-dione (1/1)

Crystal data

$C_{17}H_{13}Br_2N_3O{\cdot}C_4H_5NO_2$
M_r = 534.21
Monoclinic, $P2_1/c$
a = 9.6931 (19) Å
b = 15.699 (3) Å
c = 14.614 (3) Å
β = 108.99 (3)°
V = 2103.0 (7) Å^3
Z = 4
$F(000)$ = 1064
D_x = 1.687 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4129 reflections
θ = 3.1–26.0°
μ = 3.89 mm^{-1}
T = 293 K
Block, white
0.30 × 0.28 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR* ; Higashi, 1995)
T_{min} = 0.389, T_{max} = 0.432
16558 measured reflections
4129 independent reflections
2010 reflections with $I > 2\sigma(I)$
R_{int} = 0.125
θ_{max} = 26.0°, θ_{min} = 3.0°
h = −11→11
k = −19→19
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.148
S = 0.98
4129 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.58390 (8)	0.09771 (5)	0.60551 (6)	0.0662 (3)
Br2	0.59853 (8)	0.16358 (6)	0.40343 (6)	0.0707 (3)
O2	0.2878 (5)	0.5578 (3)	0.5158 (3)	0.0569 (13)
N2	0.1482 (5)	0.3823 (3)	0.4170 (4)	0.0384 (13)
N3	0.3233 (5)	0.2797 (3)	0.4629 (4)	0.0412 (13)
C10	−0.0753 (6)	0.2634 (4)	0.3453 (5)	0.0472 (17)
H10A	−0.1506	0.2244	0.3211	0.057*
C16	0.1779 (6)	0.2982 (4)	0.4218 (4)	0.0372 (15)
O3	0.6209 (5)	0.3572 (3)	0.6728 (4)	0.0670 (14)
C11	0.0696 (6)	0.2340 (4)	0.3875 (4)	0.0386 (15)
O1	−0.2418 (5)	0.5110 (3)	0.2818 (4)	0.0572 (13)
C8	0.0100 (6)	0.4067 (4)	0.3782 (5)	0.0408 (15)
N1	−0.0060 (5)	0.4946 (3)	0.3799 (4)	0.0431 (14)
H1A	0.0691	0.5224	0.4148	0.052*
C18	0.3969 (7)	0.5289 (4)	0.5745 (5)	0.0466 (17)
C6	−0.1117 (7)	0.6382 (4)	0.3444 (4)	0.0403 (16)
N4	0.4396 (5)	0.4441 (3)	0.5798 (4)	0.0440 (13)
H4A	0.3908	0.4057	0.5406	0.053*
C5	−0.2391 (7)	0.6855 (4)	0.3129 (5)	0.0472 (17)
H5A	−0.3286	0.6584	0.2872	0.057*
C12	0.1146 (6)	0.1482 (4)	0.3980 (5)	0.0438 (17)
C3	−0.1020 (9)	0.8141 (5)	0.3572 (6)	0.065 (2)
H3B	−0.1000	0.8733	0.3614	0.078*
C7	−0.1274 (7)	0.5432 (4)	0.3325 (5)	0.0443 (17)
C21	0.5664 (7)	0.4271 (5)	0.6533 (5)	0.0477 (17)
C15	0.3601 (6)	0.1989 (4)	0.4687 (4)	0.0397 (15)
C1	0.0213 (7)	0.6805 (4)	0.3830 (5)	0.0543 (19)
H1B	0.1075	0.6494	0.4053	0.065*
C4	−0.2326 (8)	0.7719 (5)	0.3199 (5)	0.063 (2)
H4B	−0.3187	0.8031	0.2989	0.075*
C19	0.5070 (6)	0.5760 (4)	0.6530 (5)	0.0468 (17)
H19A	0.4625	0.6011	0.6971	0.056*
H19B	0.5513	0.6209	0.6264	0.056*
C14	0.2609 (7)	0.1317 (4)	0.4380 (5)	0.0463 (17)
H14A	0.2943	0.0758	0.4447	0.056*

C2	0.0253 (8)	0.7682 (5)	0.3881 (6)	0.071 (2)
H2B	0.1143	0.7963	0.4125	0.085*
C17	0.5246 (6)	0.1862 (4)	0.5102 (5)	0.0476 (18)
H17A	0.5680	0.2398	0.5408	0.057*
C9	−0.1054 (7)	0.3486 (4)	0.3399 (5)	0.0470 (17)
H9A	−0.2005	0.3680	0.3116	0.056*
C20	0.6209 (7)	0.5095 (4)	0.7050 (5)	0.0555 (19)
H20A	0.7159	0.5240	0.7006	0.067*
H20B	0.6286	0.5056	0.7727	0.067*
C13	0.0061 (7)	0.0758 (5)	0.3690 (6)	0.070 (2)
H13A	0.0573	0.0224	0.3811	0.105*
H13B	−0.0487	0.0803	0.3014	0.105*
H13C	−0.0592	0.0786	0.4062	0.105*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0729 (5)	0.0613 (5)	0.0558 (5)	0.0189 (4)	0.0090 (4)	0.0111 (4)
Br2	0.0474 (4)	0.1006 (7)	0.0659 (6)	0.0050 (4)	0.0208 (4)	0.0021 (5)
O2	0.051 (3)	0.054 (3)	0.055 (3)	0.000 (2)	0.002 (3)	−0.002 (2)
N2	0.037 (3)	0.030 (3)	0.046 (3)	0.000 (2)	0.010 (3)	−0.001 (2)
N3	0.035 (3)	0.036 (3)	0.048 (4)	0.000 (3)	0.008 (3)	−0.001 (3)
C10	0.039 (4)	0.046 (4)	0.053 (5)	−0.010 (3)	0.009 (3)	−0.004 (3)
C16	0.035 (3)	0.038 (4)	0.040 (4)	0.001 (3)	0.014 (3)	−0.002 (3)
O3	0.068 (3)	0.054 (3)	0.069 (4)	0.009 (3)	0.009 (3)	0.006 (3)
C11	0.037 (3)	0.034 (4)	0.041 (4)	−0.001 (3)	0.008 (3)	−0.005 (3)
O1	0.042 (3)	0.053 (3)	0.063 (3)	0.009 (2)	−0.001 (3)	0.003 (3)
C8	0.039 (4)	0.039 (4)	0.043 (4)	0.006 (3)	0.011 (3)	0.004 (3)
N1	0.032 (3)	0.038 (3)	0.052 (4)	0.003 (2)	0.004 (3)	0.000 (3)
C18	0.041 (4)	0.050 (5)	0.051 (5)	−0.004 (4)	0.017 (4)	−0.003 (4)
C6	0.044 (4)	0.041 (4)	0.037 (4)	0.009 (3)	0.014 (3)	0.002 (3)
N4	0.047 (3)	0.038 (3)	0.045 (4)	−0.008 (3)	0.013 (3)	−0.006 (3)
C5	0.041 (4)	0.041 (4)	0.057 (5)	0.005 (3)	0.012 (3)	0.017 (3)
C12	0.044 (4)	0.042 (4)	0.050 (4)	−0.006 (3)	0.022 (3)	−0.007 (3)
C3	0.077 (5)	0.042 (5)	0.064 (5)	0.006 (4)	0.007 (4)	0.004 (4)
C7	0.037 (4)	0.049 (4)	0.044 (5)	0.005 (3)	0.008 (3)	0.008 (3)
C21	0.047 (4)	0.052 (5)	0.042 (4)	0.003 (4)	0.012 (4)	0.002 (4)
C15	0.042 (3)	0.041 (4)	0.035 (4)	0.004 (3)	0.009 (3)	−0.001 (3)
C1	0.046 (4)	0.044 (4)	0.063 (5)	0.006 (4)	0.004 (4)	0.007 (4)
C4	0.054 (5)	0.066 (6)	0.062 (6)	0.027 (4)	0.011 (4)	0.018 (4)
C19	0.042 (4)	0.046 (4)	0.051 (5)	−0.004 (3)	0.015 (3)	−0.005 (3)
C14	0.050 (4)	0.029 (4)	0.063 (5)	−0.002 (3)	0.023 (4)	−0.006 (3)
C2	0.062 (5)	0.050 (5)	0.078 (6)	0.001 (4)	−0.006 (4)	0.000 (4)
C17	0.043 (3)	0.036 (4)	0.052 (5)	0.006 (3)	0.001 (3)	0.000 (3)
C9	0.037 (3)	0.046 (5)	0.056 (5)	−0.002 (3)	0.012 (3)	−0.001 (4)
C20	0.046 (4)	0.062 (5)	0.051 (5)	−0.005 (4)	0.006 (4)	−0.007 (4)
C13	0.056 (5)	0.059 (5)	0.093 (7)	−0.009 (4)	0.023 (5)	−0.013 (4)

Geometric parameters (Å, º)

Br1—C17	1.918 (6)	C5—C4	1.359 (9)
Br2—C17	1.950 (7)	C5—H5A	0.9300
O2—C18	1.213 (7)	C12—C14	1.372 (8)
N2—C8	1.330 (7)	C12—C13	1.513 (9)
N2—C16	1.348 (7)	C3—C2	1.373 (10)
N3—C15	1.312 (7)	C3—C4	1.375 (10)
N3—C16	1.372 (7)	C3—H3B	0.9300
C10—C9	1.366 (8)	C21—C20	1.505 (9)
C10—C11	1.415 (8)	C15—C14	1.399 (8)
C10—H10A	0.9300	C15—C17	1.524 (8)
C16—C11	1.424 (8)	C1—C2	1.379 (9)
O3—C21	1.211 (7)	C1—H1B	0.9300
C11—C12	1.408 (8)	C4—H4B	0.9300
O1—C7	1.225 (7)	C19—C20	1.529 (8)
C8—N1	1.390 (7)	C19—H19A	0.9700
C8—C9	1.410 (8)	C19—H19B	0.9700
N1—C7	1.383 (7)	C14—H14A	0.9300
N1—H1A	0.8600	C2—H2B	0.9300
C18—N4	1.389 (8)	C17—H17A	0.9800
C18—C19	1.485 (9)	C9—H9A	0.9300
C6—C5	1.385 (8)	C20—H20A	0.9700
C6—C1	1.396 (9)	C20—H20B	0.9700
C6—C7	1.505 (8)	C13—H13A	0.9600
N4—C21	1.370 (8)	C13—H13B	0.9600
N4—H4A	0.8600	C13—H13C	0.9600
C8—N2—C16	118.2 (5)	N3—C15—C17	112.3 (5)
C15—N3—C16	116.9 (5)	C14—C15—C17	123.4 (6)
C9—C10—C11	120.5 (6)	C2—C1—C6	120.1 (6)
C9—C10—H10A	119.8	C2—C1—H1B	119.9
C11—C10—H10A	119.8	C6—C1—H1B	119.9
N2—C16—N3	113.7 (5)	C5—C4—C3	121.7 (7)
N2—C16—C11	123.7 (5)	C5—C4—H4B	119.2
N3—C16—C11	122.6 (5)	C3—C4—H4B	119.2
C12—C11—C10	125.9 (6)	C18—C19—C20	105.4 (5)
C12—C11—C16	118.2 (5)	C18—C19—H19A	110.7
C10—C11—C16	115.9 (5)	C20—C19—H19A	110.7
N2—C8—N1	112.4 (5)	C18—C19—H19B	110.7
N2—C8—C9	122.8 (6)	C20—C19—H19B	110.7
N1—C8—C9	124.8 (5)	H19A—C19—H19B	108.8
C7—N1—C8	128.3 (5)	C12—C14—C15	120.1 (6)
C7—N1—H1A	115.8	C12—C14—H14A	119.9
C8—N1—H1A	115.8	C15—C14—H14A	119.9
O2—C18—N4	125.0 (6)	C3—C2—C1	120.1 (7)
O2—C18—C19	127.0 (6)	C3—C2—H2B	120.0
N4—C18—C19	107.9 (6)	C1—C2—H2B	120.0

C5—C6—C1	119.1 (6)	C15—C17—Br1	114.3 (5)
C5—C6—C7	116.6 (6)	C15—C17—Br2	108.3 (4)
C1—C6—C7	124.3 (6)	Br1—C17—Br2	110.3 (3)
C21—N4—C18	113.9 (6)	C15—C17—H17A	107.9
C21—N4—H4A	123.0	Br1—C17—H17A	107.9
C18—N4—H4A	123.0	Br2—C17—H17A	107.9
C4—C5—C6	119.7 (6)	C10—C9—C8	118.9 (6)
C4—C5—H5A	120.1	C10—C9—H9A	120.5
C6—C5—H5A	120.1	C8—C9—H9A	120.5
C14—C12—C11	117.9 (6)	C21—C20—C19	105.0 (5)
C14—C12—C13	120.4 (6)	C21—C20—H20A	110.8
C11—C12—C13	121.7 (6)	C19—C20—H20A	110.8
C2—C3—C4	119.3 (7)	C21—C20—H20B	110.8
C2—C3—H3B	120.3	C19—C20—H20B	110.8
C4—C3—H3B	120.3	H20A—C20—H20B	108.8
O1—C7—N1	122.0 (6)	C12—C13—H13A	109.5
O1—C7—C6	121.1 (6)	C12—C13—H13B	109.5
N1—C7—C6	116.8 (6)	H13A—C13—H13B	109.5
O3—C21—N4	124.9 (6)	C12—C13—H13C	109.5
O3—C21—C20	127.3 (7)	H13A—C13—H13C	109.5
N4—C21—C20	107.8 (6)	H13B—C13—H13C	109.5
N3—C15—C14	124.4 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O2	0.86	2.22	3.060 (7)	164
N4—H4*A*···N2	0.86	2.48	3.195 (7)	141
N4—H4*A*···N3	0.86	2.27	3.098 (7)	162
C1—H1*B*···O2	0.93	2.43	3.299 (8)	156
C9—H9*A*···O1	0.93	2.30	2.870 (8)	119
C17—H17*A*···O3	0.98	2.60	3.504 (8)	154
C19—H19*B*···N3^{i}	0.97	2.58	3.538 (8)	170

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