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Methyl 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)propionate

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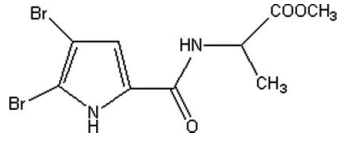
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.011 Å; R factor = 0.052; wR factor = 0.148; data-to-parameter ratio = 17.4.

The racemic title compound, $C_9H_{10}Br_2N_2O_3$, crystallizes as an inversion twin with two symmetry-independent molecules in the asymmetric unit; these are linked into pseudo-centrosymmetric dimers by intermolecular N—H···O hydrogen bonds. Weaker N—H···O hydrogen bonds link these dimers into two-dimensional layers parallel to the *ab* plane.

Related literature

For related literature, see: Banwell *et al.* (2006); Bernstein *et al.* (1995); Faulkner (2002); Marsh *et al.* (1998); Sosa *et al.* (2002); Zeng (2006); Zeng *et al.* (2007).



Experimental

Crystal data

$C_9H_{10}Br_2N_2O_3$
M_r = 354.01
Orthorhombic, $Pna2_1$
a = 15.8880 (16) Å
b = 6.1274 (6) Å
c = 24.593 (3) Å
V = 2394.2 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.77 mm^{-1}
T = 173 (2) K
0.43 × 0.40 × 0.26 mm

Data collection

Bruker SMART 1 K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.159, T_{max} = 0.272
(expected range = 0.101–0.172)
18530 measured reflections
5111 independent reflections
4233 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.148
S = 1.09
5111 reflections
294 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}
Absolute structure: Flack (1983), with 2453 Friedel pairs
Flack parameter: 0.592 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O2^{i}	0.88	2.25	3.122 (8)	169
N3—H3A···O1	0.88	1.93	2.784 (8)	162
N2—H2···O5^{ii}	0.88	2.26	3.127 (8)	168
N1—H1···O4	0.88	1.88	2.734 (8)	164

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2266).

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supplementary materials

Acta Cryst. (2007). E**63**, o3424 [**doi:10.1107/S1600536807032497**]

Methyl 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)propionate

X.-C. Zeng, J. Zeng, X. Li and X. Ling

Comment

Pyrrole derivatives are well known in many marine organisms (Faulkner, 2002), some show important bioactivities, such as antitumor activity (Banwell *et al.*, 2006) and protein kinase inhibiting activity (Sosa *et al.*, 2002). This is the reason why they have attracted our interest. This study follows our previous studies on (*S*)-Methyl 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)-3-methylbutanoate (Zeng, 2006) and Methyl 3-(3,4,5-tribromo-1*H*-pyrrol-2-ylcarboxamido)propionate (Zeng *et al.*, 2007).

In the crystal structure, the two independent molecules are disposed over a false center of inversion (Fig. 1); this feature has been noted in compounds beloning to the $Pna2_1$ group (Marsh *et al.*, 1998). These two molecules being R– and S-enantiomers are linked through N1—H···O4 and N3—H···O1 hydrogen bonds (Table 1) to form pseudo-centrosymmetric dimer (also shown in Fig. 1), which graph-set analysis describes as an $R_2^2(10)$ motif (Bernstein *et al.*, 1995). At the same time, the weaker N2—H···O5 and N4—H···O2 hydrogen bonds link the dimers into two-dimensional layers parallel to *ab*-plane (Fig. 2).

Experimental

The hydrochloric acid salt of DL-methyl 2-aminopropionate (0.70 g, 5 mmol) and 4,5-dibromo-2-trichloroacetylpyrrole (1.85 g, 5 mmol) were added to 12 ml of acetonitrile, followed by the dropwise addition of triethylamine (1.4 ml). The mixture was stirred at room temperature for 8 h, and then poured into water. After filtration, the precipitate was collected as a pale yellow solid. The impure product was dissolved in ethanol at room temperature. Colourless crystals suitable for X-ray analysis (m. p. 485 K, in 81.4% yield) grew over a period of several days when the solution was exposed to air. CH&N elemental analysis. Calc. for $C_9H_{10}Br_2N_2O_3$: C 30.54, H 2.85, N 7.91%; found: C 30.27, H 2.69, N 8.07%.

Refinement

The H atoms were positioned geometrically [C—H = 1.00 Å for CH, 0.98 Å for CH_3, C—H = 0.95 Å for CH(aromatic), and N—H = 0.88 Å] and refined using a riding model, with $U_{iso} = 1.2U_{eq}$ ($1.5U_{eq}$ for the methyl group) of the parent atom. The highest residual peak [2.35 e $Å^{-3}$] is situated 0.97 Å at Br4 atom.

Because of racemic twinning, the TWIN and BASF instructions were used in the final refinement.

Figures

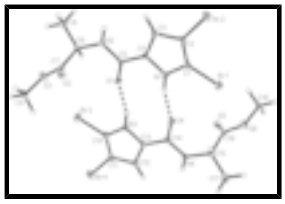

Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

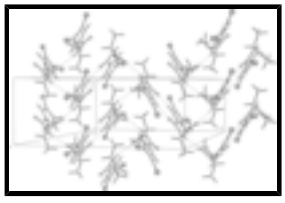

Fig. 2. The crystal packing of (I), showing the two-dimensional network formed by hydrogen bonds (dashed lines).

Methyl 2-(4,5-dibromo-1*H*-pyrrole-2-carboxamido)propionate

Crystal data

$C_9H_{10}Br_2N_2O_3$	D_x = 1.964 Mg m^{-3}
M_r = 354.01	Melting point: 485 K
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 5810 reflections
a = 15.8880 (16) Å	θ = 2.6–26.8º
b = 6.1274 (6) Å	μ = 6.77 mm^{-1}
c = 24.593 (3) Å	*T* = 173 (2) K
V = 2394.2 (4) Å^3	Plate, colourless
Z = 8	0.43 × 0.40 × 0.26 mm
F_{000} = 1376	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	5111 independent reflections
Radiation source: fine-focus sealed tube	4233 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.053
T = 173(2) K	θ_{max} = 27.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −20→20
T_{min} = 0.159, T_{max} = 0.272	*k* = −7→7
18530 measured reflections	*l* = −30→31

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.148$

$S = 1.09$

5111 reflections

294 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0945P)^2 + 0.3872P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 2.35$ e Å^{-3}

$\Delta\rho_{min} = -0.88$ e Å^{-3}

Extinction correction: none

Absolute structure: Flack (1983), 2453 Friedel pairs

Flack parameter: 0.592 (16)

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 $F^2 > 2$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}
Br4	0.47977 (6)	0.33319 (16)	0.71923 (3)	0.0387 (2)
Br3	0.36898 (6)	−0.12861 (15)	0.66069 (4)	0.0396 (2)
C12	0.4929 (5)	0.3982 (13)	0.6001 (4)	0.0233 (16)
H12	0.5234	0.5315	0.6017	0.028*
O4	0.4423 (3)	0.2217 (9)	0.4619 (2)	0.0237 (12)
C17	0.5665 (5)	0.7947 (12)	0.4204 (4)	0.0285 (18)
H17A	0.6201	0.8080	0.4399	0.043*
H17B	0.5255	0.8965	0.4360	0.043*
H17C	0.5751	0.8293	0.3819	0.043*
C14	0.4777 (4)	0.3376 (12)	0.4973 (3)	0.0180 (15)
N4	0.5247 (4)	0.5104 (10)	0.4832 (3)	0.0191 (13)
H4	0.5496	0.5890	0.5085	0.023*
C10	0.4226 (5)	0.0981 (13)	0.6243 (3)	0.0211 (15)
C15	0.5345 (4)	0.5679 (13)	0.4257 (3)	0.0205 (15)
H15	0.4781	0.5591	0.4077	0.025*
C11	0.4642 (5)	0.2747 (13)	0.6445 (3)	0.0251 (17)
N3	0.4262 (4)	0.1053 (10)	0.5702 (3)	0.0199 (13)
H3A	0.4048	0.0075	0.5480	0.024*
C13	0.4689 (4)	0.2907 (12)	0.5548 (3)	0.0187 (15)
O5	0.6450 (4)	0.2933 (9)	0.4192 (2)	0.0271 (12)
O6	0.5853 (4)	0.4267 (9)	0.3443 (2)	0.0275 (12)

C16	0.5944 (4)	0.4079 (11)	0.3973 (3)	0.0172 (14)
C18	0.6420 (6)	0.2931 (16)	0.3116 (4)	0.036 (2)
H18A	0.6316	0.1385	0.3193	0.054*
H18B	0.7004	0.3292	0.3207	0.054*
H18C	0.6320	0.3219	0.2730	0.054*
Br1	0.40261 (6)	0.14472 (15)	0.32146 (4)	0.0364 (2)
Br2	0.27815 (6)	−0.30292 (15)	0.26376 (3)	0.0382 (2)
C3	0.2788 (5)	−0.3833 (13)	0.3805 (3)	0.0227 (16)
H3	0.2475	−0.5152	0.3789	0.027*
C5	0.3026 (4)	−0.3344 (11)	0.4843 (3)	0.0162 (14)
C2	0.3038 (5)	−0.2547 (14)	0.3366 (3)	0.0251 (17)
N2	0.2550 (4)	−0.5115 (10)	0.4979 (2)	0.0210 (13)
H2	0.2306	−0.5897	0.4723	0.025*
C6	0.2446 (5)	−0.5711 (12)	0.5552 (3)	0.0203 (15)
H6	0.3004	−0.5624	0.5740	0.024*
N1	0.3516 (4)	−0.0987 (10)	0.4115 (2)	0.0184 (12)
H1	0.3768	−0.0064	0.4335	0.022*
C4	0.3084 (5)	−0.2816 (13)	0.4269 (3)	0.0202 (15)
O1	0.3378 (3)	−0.2291 (9)	0.5192 (2)	0.0252 (12)
O2	0.1322 (4)	−0.2991 (9)	0.5614 (2)	0.0269 (12)
C7	0.1833 (5)	−0.4166 (12)	0.5826 (3)	0.0202 (15)
O3	0.1928 (4)	−0.4370 (10)	0.6358 (2)	0.0306 (13)
C9	0.1369 (6)	−0.3109 (15)	0.6690 (3)	0.033 (2)
H9A	0.1523	−0.1564	0.6667	0.049*
H9B	0.1411	−0.3600	0.7068	0.049*
H9C	0.0790	−0.3302	0.6561	0.049*
C1	0.3490 (5)	−0.0837 (13)	0.3566 (3)	0.0223 (15)
C8	0.2118 (6)	−0.8018 (13)	0.5586 (4)	0.0299 (19)
H8A	0.1564	−0.8097	0.5412	0.045*
H8B	0.2068	−0.8449	0.5968	0.045*
H8C	0.2508	−0.9004	0.5400	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br4	0.0490 (5)	0.0491 (5)	0.0180 (4)	−0.0051 (4)	−0.0040 (4)	−0.0074 (4)
Br3	0.0530 (6)	0.0371 (5)	0.0288 (5)	−0.0080 (4)	0.0053 (4)	0.0061 (4)
C12	0.020 (3)	0.023 (4)	0.027 (4)	−0.001 (3)	0.003 (3)	−0.004 (3)
O4	0.031 (3)	0.022 (3)	0.018 (3)	−0.009 (2)	−0.003 (2)	−0.002 (2)
C17	0.036 (4)	0.021 (4)	0.028 (4)	0.001 (3)	−0.003 (3)	0.000 (3)
C14	0.018 (3)	0.018 (3)	0.018 (4)	0.006 (3)	0.003 (3)	−0.001 (3)
N4	0.018 (3)	0.018 (3)	0.022 (3)	−0.003 (2)	0.004 (2)	−0.005 (2)
C10	0.023 (4)	0.026 (4)	0.014 (4)	0.002 (3)	0.001 (3)	0.003 (3)
C15	0.018 (3)	0.025 (4)	0.019 (4)	0.004 (3)	0.003 (3)	0.000 (3)
C11	0.025 (4)	0.034 (4)	0.016 (4)	0.000 (3)	−0.002 (3)	−0.004 (3)
N3	0.017 (3)	0.024 (3)	0.019 (3)	−0.002 (2)	0.001 (3)	−0.001 (3)
C13	0.013 (3)	0.016 (4)	0.027 (4)	0.006 (3)	0.004 (3)	0.001 (3)
O5	0.033 (3)	0.025 (3)	0.023 (3)	0.010 (2)	0.001 (2)	0.004 (2)

O6	0.037 (3)	0.031 (3)	0.015 (3)	0.016 (3)	0.002 (2)	0.000 (2)
C16	0.021 (3)	0.015 (3)	0.016 (3)	0.001 (3)	0.002 (3)	−0.001 (3)
C18	0.043 (5)	0.047 (5)	0.018 (5)	0.021 (4)	0.011 (4)	−0.001 (4)
Br1	0.0495 (5)	0.0368 (5)	0.0231 (4)	−0.0152 (4)	−0.0014 (4)	0.0042 (4)
Br2	0.0462 (5)	0.0514 (5)	0.0172 (4)	−0.0163 (4)	−0.0014 (4)	−0.0087 (4)
C3	0.025 (4)	0.021 (4)	0.022 (4)	−0.010 (3)	0.001 (3)	−0.007 (3)
C5	0.015 (3)	0.013 (3)	0.021 (4)	−0.001 (3)	0.004 (3)	−0.004 (3)
C2	0.029 (4)	0.030 (4)	0.016 (4)	−0.005 (4)	0.000 (3)	−0.010 (3)
N2	0.028 (3)	0.017 (3)	0.018 (3)	−0.005 (2)	0.004 (3)	−0.005 (2)
C6	0.020 (3)	0.015 (4)	0.025 (4)	−0.001 (3)	−0.001 (3)	−0.002 (3)
N1	0.021 (3)	0.019 (3)	0.015 (3)	−0.005 (2)	−0.004 (2)	−0.002 (2)
C4	0.027 (4)	0.027 (4)	0.007 (3)	−0.007 (3)	0.003 (3)	−0.004 (3)
O1	0.032 (3)	0.022 (3)	0.021 (3)	−0.010 (2)	−0.002 (2)	−0.002 (2)
O2	0.036 (3)	0.026 (3)	0.019 (3)	0.008 (2)	0.000 (2)	0.003 (2)
C7	0.025 (4)	0.016 (3)	0.020 (4)	−0.004 (3)	0.002 (3)	0.002 (3)
O3	0.041 (3)	0.034 (3)	0.016 (3)	0.013 (3)	0.002 (2)	0.010 (2)
C9	0.043 (5)	0.042 (5)	0.013 (4)	0.013 (4)	0.011 (4)	0.001 (3)
C1	0.025 (4)	0.028 (4)	0.014 (4)	−0.006 (3)	0.002 (3)	0.001 (3)
C8	0.037 (5)	0.018 (4)	0.035 (5)	−0.003 (3)	0.001 (4)	0.008 (3)

Geometric parameters (Å, °)

Br4—C11	1.889 (8)	Br1—C1	1.853 (7)
Br3—C10	1.859 (8)	Br2—C2	1.861 (8)
C12—C13	1.350 (12)	C3—C4	1.382 (10)
C12—C11	1.404 (12)	C3—C2	1.394 (12)
C12—H12	0.9500	C3—H3	0.9500
O4—C14	1.256 (9)	C5—O1	1.210 (9)
C17—C15	1.486 (11)	C5—N2	1.364 (9)
C17—H17A	0.9800	C5—C4	1.451 (10)
C17—H17B	0.9800	C2—C1	1.362 (11)
C17—H17C	0.9800	N2—C6	1.467 (10)
C14—N4	1.341 (9)	N2—H2	0.8800
C14—C13	1.450 (11)	C6—C8	1.509 (10)
N4—C15	1.468 (10)	C6—C7	1.516 (10)
N4—H4	0.8800	C6—H6	1.0000
C10—N3	1.332 (10)	N1—C1	1.352 (10)
C10—C11	1.362 (11)	N1—C4	1.368 (10)
C15—C16	1.534 (10)	N1—H1	0.8800
C15—H15	1.0000	O2—C7	1.203 (9)
N3—C13	1.376 (10)	C7—O3	1.322 (9)
N3—H3A	0.8800	O3—C9	1.433 (10)
O5—C16	1.196 (9)	C9—H9A	0.9800
O6—C16	1.317 (9)	C9—H9B	0.9800
O6—C18	1.458 (9)	C9—H9C	0.9800
C18—H18A	0.9800	C8—H8A	0.9800
C18—H18B	0.9800	C8—H8B	0.9800
C18—H18C	0.9800	C8—H8C	0.9800
C13—C12—C11	106.6 (7)	C4—C3—C2	106.7 (7)

C13—C12—H12	126.7	C4—C3—H3	126.6
C11—C12—H12	126.7	C2—C3—H3	126.6
C15—C17—H17A	109.5	O1—C5—N2	120.4 (7)
C15—C17—H17B	109.5	O1—C5—C4	122.8 (7)
H17A—C17—H17B	109.5	N2—C5—C4	116.8 (6)
C15—C17—H17C	109.5	C1—C2—C3	107.8 (7)
H17A—C17—H17C	109.5	C1—C2—Br2	125.8 (6)
H17B—C17—H17C	109.5	C3—C2—Br2	126.4 (6)
O4—C14—N4	121.1 (7)	C5—N2—C6	119.7 (6)
O4—C14—C13	121.4 (7)	C5—N2—H2	120.1
N4—C14—C13	117.5 (7)	C6—N2—H2	120.1
C14—N4—C15	119.9 (6)	N2—C6—C8	109.0 (6)
C14—N4—H4	120.1	N2—C6—C7	110.1 (6)
C15—N4—H4	120.1	C8—C6—C7	109.8 (6)
N3—C10—C11	108.5 (7)	N2—C6—H6	109.3
N3—C10—Br3	121.7 (6)	C8—C6—H6	109.3
C11—C10—Br3	129.9 (6)	C7—C6—H6	109.3
N4—C15—C17	110.2 (7)	C1—N1—C4	108.5 (6)
N4—C15—C16	110.5 (6)	C1—N1—H1	125.8
C17—C15—C16	110.2 (6)	C4—N1—H1	125.8
N4—C15—H15	108.6	N1—C4—C3	108.1 (7)
C17—C15—H15	108.6	N1—C4—C5	119.0 (6)
C16—C15—H15	108.6	C3—C4—C5	132.9 (7)
C10—C11—C12	107.6 (7)	O2—C7—O3	124.1 (7)
C10—C11—Br4	124.7 (6)	O2—C7—C6	128.0 (7)
C12—C11—Br4	127.7 (6)	O3—C7—C6	107.9 (6)
C10—N3—C13	108.8 (7)	C7—O3—C9	116.2 (6)
C10—N3—H3A	125.6	O3—C9—H9A	109.5
C13—N3—H3A	125.6	O3—C9—H9B	109.5
C12—C13—N3	108.4 (7)	H9A—C9—H9B	109.5
C12—C13—C14	132.9 (7)	O3—C9—H9C	109.5
N3—C13—C14	118.6 (7)	H9A—C9—H9C	109.5
C16—O6—C18	115.4 (6)	H9B—C9—H9C	109.5
O5—C16—O6	124.8 (7)	N1—C1—C2	108.9 (7)
O5—C16—C15	126.0 (7)	N1—C1—Br1	120.2 (6)
O6—C16—C15	109.1 (6)	C2—C1—Br1	130.9 (6)
O6—C18—H18A	109.5	C6—C8—H8A	109.5
O6—C18—H18B	109.5	C6—C8—H8B	109.5
H18A—C18—H18B	109.5	H8A—C8—H8B	109.5
O6—C18—H18C	109.5	C6—C8—H8C	109.5
H18A—C18—H18C	109.5	H8A—C8—H8C	109.5
H18B—C18—H18C	109.5	H8B—C8—H8C	109.5
O4—C14—N4—C15	0.8 (10)	C4—C3—C2—C1	1.4 (9)
C13—C14—N4—C15	−178.8 (6)	C4—C3—C2—Br2	−177.2 (6)
C14—N4—C15—C17	163.4 (6)	O1—C5—N2—C6	1.6 (11)
C14—N4—C15—C16	−74.6 (8)	C4—C5—N2—C6	−178.5 (7)
N3—C10—C11—C12	1.4 (9)	C5—N2—C6—C8	−163.9 (7)
Br3—C10—C11—C12	−179.7 (6)	C5—N2—C6—C7	75.7 (8)
N3—C10—C11—Br4	−178.0 (6)	C1—N1—C4—C3	0.4 (9)

Br3—C10—C11—Br4	0.9 (11)	C1—N1—C4—C5	179.6 (7)
C13—C12—C11—C10	−0.9 (9)	C2—C3—C4—N1	−1.1 (9)
C13—C12—C11—Br4	178.5 (6)	C2—C3—C4—C5	179.8 (9)
C11—C10—N3—C13	−1.4 (9)	O1—C5—C4—N1	−3.6 (12)
Br3—C10—N3—C13	179.6 (5)	N2—C5—C4—N1	176.5 (6)
C11—C12—C13—N3	0.1 (8)	O1—C5—C4—C3	175.4 (8)
C11—C12—C13—C14	178.1 (8)	N2—C5—C4—C3	−4.5 (13)
C10—N3—C13—C12	0.8 (8)	N2—C6—C7—O2	18.8 (11)
C10—N3—C13—C14	−177.6 (6)	C8—C6—C7—O2	−101.1 (10)
O4—C14—C13—C12	−172.8 (8)	N2—C6—C7—O3	−163.4 (6)
N4—C14—C13—C12	6.9 (12)	C8—C6—C7—O3	76.6 (8)
O4—C14—C13—N3	5.1 (10)	O2—C7—O3—C9	0.9 (12)
N4—C14—C13—N3	−175.2 (6)	C6—C7—O3—C9	−177.0 (7)
C18—O6—C16—O5	0.7 (12)	C4—N1—C1—C2	0.5 (9)
C18—O6—C16—C15	176.5 (7)	C4—N1—C1—Br1	−179.3 (5)
N4—C15—C16—O5	−20.3 (11)	C3—C2—C1—N1	−1.2 (10)
C17—C15—C16—O5	101.7 (9)	Br2—C2—C1—N1	177.4 (6)
N4—C15—C16—O6	163.9 (6)	C3—C2—C1—Br1	178.5 (6)
C17—C15—C16—O6	−74.1 (8)	Br2—C2—C1—Br1	−2.9 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O2^{i}	0.88	2.25	3.122 (8)	169
N3—H3A···O1	0.88	1.93	2.784 (8)	162
N2—H2···O5^{ii}	0.88	2.26	3.127 (8)	168
N1—H1···O4	0.88	1.88	2.734 (8)	164

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

Fig. 1

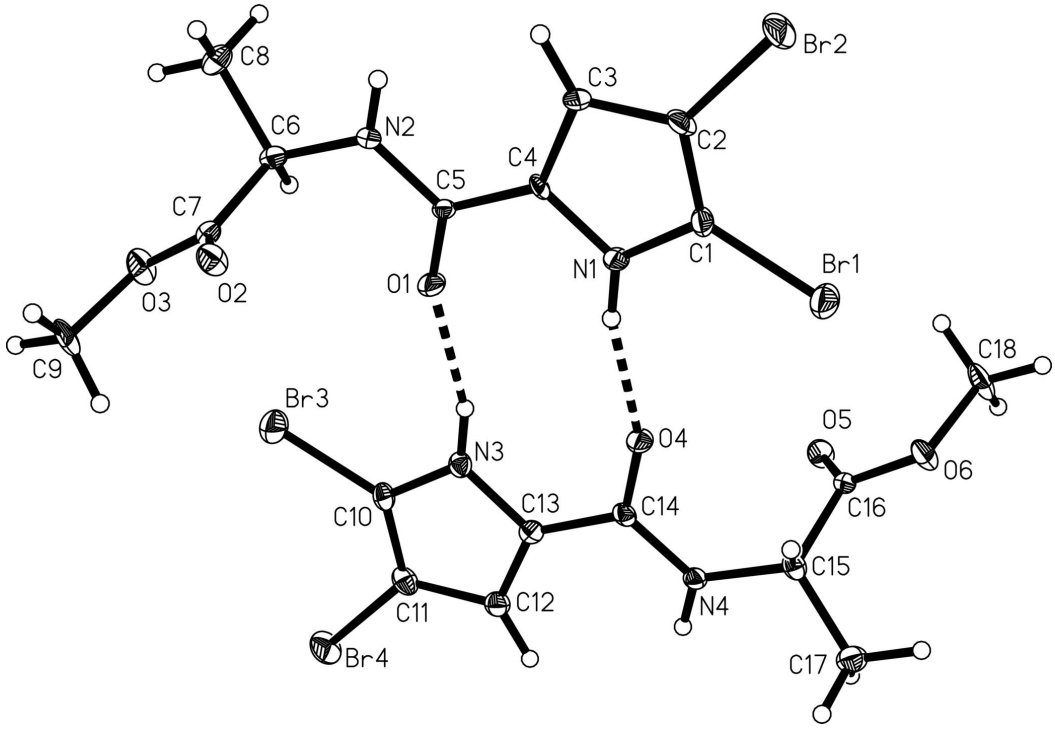
C8
C6
N2
C5
C4
C3
Br2
C2
C7
O1
N1
C1
Br1
O3
O2
C9
C18
Br3
N3
O4
O5
O6
C10
C13
C14
C16
C15
C11
C12
N4
Br4
C17

Fig. 2