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Phthalazin-1(2*H*)-one–picric acid (1/1)

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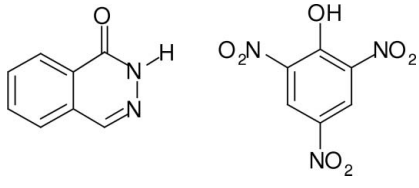
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.091; data-to-parameter ratio = 11.1.

The geometric parameters of the title compound, $C_8H_6N_2O{\cdot}C_6H_3N_3O_7$, are in the usual ranges. The three nitro groups are almost coplanar with the aromatic picrate ring [dihedral angles 10.2 (2)°, 7.62 (16) and 8.08 (17)°]. The molecular conformation of the picric acid is stabilized by an intramolecular O—H···O hydrogen bond. The phthalazin-1(2*H*)-one molecules are connected *via* N—H···O hydrogen bonds, forming centrosymmetric dimers.

Related literature

For related literature, see: Büyükgüngör, Odabaşoğlu, Narayana, *et al.* (2007); Büyükgüngör, Odabaşoğlu, Vijesh & Yathirajan (2007); Balogh-Hergovich *et al.* (1997); Butcher *et al.* (2007); Cheng *et al.* (1999); Coates (1999); Harrison *et al.* (2007); Li *et al.* (2006); Porter (1979); Sarojini *et al.* (2007); Shubin *et al.* (2004); Yatani *et al.* (2001).



Experimental

Crystal data

$C_6H_3N_3O_7{\cdot}C_8H_6N_2O$
M_r = 375.26
Monoclinic, $P2_1/n$
a = 6.9277 (4) Å
b = 9.2087 (8) Å
c = 23.6900 (15) Å
β = 95.246 (5)°
V = 1504.98 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 173 (2) K
0.27 × 0.25 × 0.24 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: none
18938 measured reflections
2819 independent reflections
2384 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.091
S = 1.02
2819 reflections
253 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.94 (2)	1.89 (2)	2.8252 (16)	175.2 (17)
O11—H11···O17	0.90 (3)	1.79 (3)	2.5819 (16)	146 (2)

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2514).

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supplementary materials

Acta Cryst. (2008). E**64**, o119 [**doi:10.1107/S1600536807063362**]

Phthalazin-1(2*H*)-one-picric acid (1/1)

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Comment

Phthalazines, also called benzo-orthodiazines or benzopyridazines, are a group of heterocyclic compounds isomeric with the cinnolines. The practical interest upon phthalazine derivatives is based on their widespread applications (Coates, 1999). Phthalazines, like others members of the isomeric diazine series, have found wide applications as therapeutic agents (Porter, 1979). Phthalazines are also commonly used as ligands in transition metal catalysis (Balogh-Hergovich *et al.*, 1997 & Yatani *et al.*, 2001), as chemiluminescent materials (Shubin *et al.*, 2004) and for optical applications (Cheng *et al.*, 1999). 2-Substituted-8-(4,6-dimethoxypyrimidin-2-yloxy)-4-methylphthalazin-1-one derivatives are used as herbicides (Li *et al.*, 2006). Structures of phthalazin-1(2*H*)-one (

Büyükgüngör, Odabaşoğlu, Narayana, Vijesh & Yathirajan, 2007), (1*Z*)-phthalazin-1(2*H*)-one isopropylidenehydrazone (Büyükgüngör, Odabaşoğlu, Vijesh & Yathirajan, 2007), 4-methoxybenzaldehyde (phthalazin-1-ylidene)hydrazone (Butcher *et al.*, 2007) have been published. A similar structure was observed with phenothiazine-picric acid (Harrison *et al.*, 2007). In continuation to our studies on the structures of picrates (Sarojini *et al.*, 2007), a new cocrystal of phthalazin-1(2*H*)-one with picric acid was obtained when we prepared the picrate using the usual procedure and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. The three nitrogroups are almost coplanar with the aromatic picrate ring [dihedral angles 10.2 (2)°, 7.62 (16) and 8.08 (17)°]. The molecular conformation of the picric acid is stabilized by an intramolecular O—H···O hydrogen bond. The phthalazin-1(2*H*)-one molecules are connected *via* N—-H···O hydrogen bonds to form centrosymmetric dimers.

Experimental

Phthalazin-1(2*H*)-one (1.46 g, 0.01 mol) was dissolved in 25 ml of ethanol. Picric acid (2.29 g, 0.01 mol) was dissolved in 10 ml of water. Both the solutions were mixed and to this 5 ml of 5 *M* HCl was added and stirred for few minutes. The precipitate formed was filtered, dried and *x*-ray quality crystals were obtained by slow evaporation from absolute ethanol [m. p.: 403–405 K]. Composition: Found (Calculated): C 44.72 (44.81), H 2.39 (2.42), N 18.60% (18.66%).

Refinement

H atoms were found in a difference map, but those bonded to C were geometrically positioned and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2 U_{eq}(C)] using a riding model with C—H = 0.95 Å. H atoms bonded to N and O were freely refined.

Figures

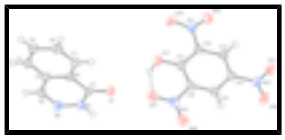


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. The intramolecular hydrogen bond is shown as a dashed line.

Phthalazin-1(2*H*)-one–picric acid (1/1)

Crystal data

$C_6H_3N_3O_7 \cdot C_8H_6N_2O$	$F_{000} = 768$
$M_r = 375.26$	$D_x = 1.656$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 18866 reflections
$a = 6.9277$ (4) Å	$\theta = 3.5$–25.7º
$b = 9.2087$ (8) Å	$\mu = 0.14$ mm^{-1}
$c = 23.6900$ (15) Å	$T = 173$ (2) K
$\beta = 95.246$ (5)º	Block, yellow
$V = 1504.98$ (18) Å^3	0.27 × 0.25 × 0.24 mm
$Z = 4$	

Data collection

Stoe IPDSII diffractometer	2384 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.043$
Monochromator: graphite	$\theta_{max} = 25.6$º
$T = 173$(2) K	$\theta_{min} = 3.4$º
ω scans	$h = -8 \rightarrow 8$
Absorption correction: none	$k = -11 \rightarrow 11$
18938 measured reflections	$l = -28 \rightarrow 28$
2819 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.034$	$w = 1/[\sigma^2(F_o^2) + (0.0623P)^2 + 0.1404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2819 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}

253 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL, $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0119 (17)

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.66147 (14)	0.65518 (11)	0.51988 (4)	0.0300 (2)
N1	0.67645 (17)	0.48688 (13)	0.45056 (5)	0.0272 (3)
H1	0.562 (3)	0.445 (2)	0.4613 (8)	0.044 (5)*
N2	0.75780 (17)	0.41599 (13)	0.40757 (5)	0.0292 (3)
C1	0.74820 (18)	0.60533 (15)	0.48045 (5)	0.0240 (3)
C2	0.9215 (2)	0.46716 (16)	0.39350 (6)	0.0287 (3)
H2	0.9818	0.4186	0.3644	0.034*
C3	1.01736 (19)	0.59266 (15)	0.41912 (6)	0.0258 (3)
C4	1.1946 (2)	0.64606 (17)	0.40233 (6)	0.0303 (3)
H4	1.2568	0.5978	0.3735	0.036*
C5	1.2770 (2)	0.76868 (17)	0.42798 (6)	0.0318 (3)
H5	1.3962	0.8044	0.4167	0.038*
C6	1.1867 (2)	0.84098 (16)	0.47044 (6)	0.0310 (3)
H6	1.2441	0.9261	0.4873	0.037*
C7	1.0148 (2)	0.78938 (15)	0.48800 (6)	0.0271 (3)
H7	0.9549	0.8380	0.5172	0.033*
C8	0.92916 (18)	0.66482 (15)	0.46255 (5)	0.0236 (3)
C11	0.55633 (18)	0.74695 (14)	0.68594 (6)	0.0240 (3)
C12	0.58222 (18)	0.69094 (14)	0.74195 (6)	0.0235 (3)
C13	0.44722 (18)	0.71095 (14)	0.78092 (6)	0.0239 (3)
H13	0.4688	0.6721	0.8181	0.029*
C14	0.28010 (19)	0.78865 (14)	0.76467 (6)	0.0241 (3)
C15	0.24542 (19)	0.84793 (14)	0.71086 (6)	0.0249 (3)
H15	0.1298	0.9006	0.7003	0.030*
C16	0.38311 (19)	0.82836 (14)	0.67310 (6)	0.0242 (3)
N11	0.75280 (16)	0.60220 (13)	0.76171 (5)	0.0280 (3)
N12	0.13440 (16)	0.80502 (13)	0.80526 (5)	0.0279 (3)
N13	0.34405 (18)	0.89697 (13)	0.61722 (5)	0.0287 (3)

O11	0.68359 (15)	0.71926 (12)	0.64906 (5)	0.0332 (3)
H11	0.643 (4)	0.767 (3)	0.6170 (11)	0.075 (7)*
O12	0.89061 (14)	0.59522 (13)	0.73298 (5)	0.0405 (3)
O13	0.74780 (16)	0.53924 (14)	0.80712 (5)	0.0434 (3)
O14	0.15798 (15)	0.73720 (13)	0.84986 (4)	0.0392 (3)
O15	−0.00576 (15)	0.88503 (13)	0.79219 (5)	0.0397 (3)
O16	0.18568 (17)	0.95344 (12)	0.60558 (5)	0.0410 (3)
O17	0.47424 (16)	0.89587 (12)	0.58474 (4)	0.0374 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0242 (5)	0.0360 (6)	0.0314 (5)	−0.0009 (4)	0.0101 (4)	−0.0075 (4)
N1	0.0236 (6)	0.0319 (6)	0.0271 (6)	−0.0020 (5)	0.0077 (5)	−0.0047 (5)
N2	0.0285 (6)	0.0324 (6)	0.0277 (6)	0.0001 (5)	0.0073 (5)	−0.0043 (5)
C1	0.0201 (6)	0.0283 (7)	0.0237 (6)	0.0036 (5)	0.0021 (5)	0.0005 (5)
C2	0.0292 (7)	0.0329 (7)	0.0250 (7)	0.0025 (6)	0.0083 (5)	−0.0028 (6)
C3	0.0238 (6)	0.0303 (7)	0.0234 (7)	0.0036 (5)	0.0033 (5)	0.0041 (5)
C4	0.0271 (7)	0.0381 (8)	0.0270 (7)	0.0036 (6)	0.0090 (6)	0.0049 (6)
C5	0.0238 (7)	0.0401 (8)	0.0322 (8)	−0.0028 (6)	0.0056 (6)	0.0082 (6)
C6	0.0278 (7)	0.0317 (7)	0.0329 (8)	−0.0031 (6)	−0.0006 (6)	0.0037 (6)
C7	0.0249 (6)	0.0301 (7)	0.0262 (7)	0.0028 (5)	0.0020 (5)	−0.0007 (5)
C8	0.0192 (6)	0.0291 (7)	0.0226 (6)	0.0031 (5)	0.0024 (5)	0.0030 (5)
C11	0.0225 (6)	0.0228 (6)	0.0271 (7)	−0.0038 (5)	0.0045 (5)	−0.0047 (5)
C12	0.0193 (6)	0.0234 (6)	0.0275 (7)	−0.0001 (5)	0.0010 (5)	−0.0035 (5)
C13	0.0234 (6)	0.0238 (6)	0.0242 (7)	−0.0013 (5)	0.0007 (5)	−0.0018 (5)
C14	0.0211 (6)	0.0248 (6)	0.0269 (7)	−0.0010 (5)	0.0054 (5)	−0.0035 (5)
C15	0.0227 (6)	0.0223 (6)	0.0292 (7)	0.0000 (5)	0.0006 (5)	−0.0024 (5)
C16	0.0271 (7)	0.0213 (6)	0.0240 (7)	−0.0025 (5)	0.0010 (5)	−0.0009 (5)
N11	0.0232 (6)	0.0320 (6)	0.0282 (6)	0.0030 (5)	−0.0003 (5)	−0.0058 (5)
N12	0.0239 (6)	0.0298 (6)	0.0306 (6)	0.0008 (5)	0.0064 (5)	−0.0022 (5)
N13	0.0360 (7)	0.0248 (6)	0.0250 (6)	−0.0001 (5)	0.0015 (5)	−0.0017 (5)
O11	0.0300 (5)	0.0421 (6)	0.0291 (6)	0.0055 (4)	0.0108 (4)	0.0008 (5)
O12	0.0228 (5)	0.0580 (7)	0.0415 (6)	0.0097 (5)	0.0079 (4)	−0.0005 (5)
O13	0.0417 (6)	0.0551 (7)	0.0337 (6)	0.0212 (5)	0.0044 (5)	0.0100 (5)
O14	0.0337 (6)	0.0549 (7)	0.0304 (6)	0.0046 (5)	0.0101 (4)	0.0094 (5)
O15	0.0321 (6)	0.0410 (6)	0.0478 (7)	0.0143 (5)	0.0132 (5)	0.0035 (5)
O16	0.0471 (7)	0.0412 (6)	0.0336 (6)	0.0164 (5)	−0.0028 (5)	0.0029 (5)
O17	0.0432 (6)	0.0420 (6)	0.0280 (5)	−0.0031 (5)	0.0087 (5)	0.0034 (4)

Geometric parameters (Å, °)

O1—C1	1.2438 (17)	C11—C12	1.4198 (19)
N1—C1	1.3688 (18)	C11—C16	1.4240 (19)
N1—N2	1.3733 (16)	C12—C13	1.385 (2)
N1—H1	0.94 (2)	C12—N11	1.4772 (17)
N2—C2	1.2990 (19)	C13—C14	1.3853 (19)
C1—C8	1.4659 (19)	C13—H13	0.9500
C2—C3	1.439 (2)	C14—C15	1.387 (2)

C2—H2	0.9500	C14—N12	1.4640 (18)
C3—C8	1.4102 (19)	C15—C16	1.378 (2)
C3—C4	1.413 (2)	C15—H15	0.9500
C4—C5	1.381 (2)	C16—N13	1.4694 (17)
C4—H4	0.9500	N11—O12	1.2238 (16)
C5—C6	1.400 (2)	N11—O13	1.2255 (17)
C5—H5	0.9500	N12—O14	1.2255 (16)
C6—C7	1.381 (2)	N12—O15	1.2356 (16)
C6—H6	0.9500	N13—O16	1.2226 (16)
C7—C8	1.4019 (19)	N13—O17	1.2381 (17)
C7—H7	0.9500	O11—H11	0.90 (3)
C11—O11	1.3214 (17)		
C1—N1—N2	127.46 (12)	O11—C11—C12	120.86 (12)
C1—N1—H1	117.8 (11)	O11—C11—C16	124.09 (13)
N2—N1—H1	114.7 (11)	C12—C11—C16	115.01 (12)
C2—N2—N1	116.41 (12)	C13—C12—C11	122.63 (12)
O1—C1—N1	120.34 (12)	C13—C12—N11	115.59 (12)
O1—C1—C8	124.33 (12)	C11—C12—N11	121.74 (12)
N1—C1—C8	115.34 (12)	C12—C13—C14	118.79 (12)
N2—C2—C3	124.27 (13)	C12—C13—H13	120.6
N2—C2—H2	117.9	C14—C13—H13	120.6
C3—C2—H2	117.9	C13—C14—C15	121.91 (13)
C8—C3—C4	119.14 (13)	C13—C14—N12	118.66 (12)
C8—C3—C2	118.16 (12)	C15—C14—N12	119.41 (12)
C4—C3—C2	122.69 (13)	C16—C15—C14	118.24 (12)
C5—C4—C3	119.70 (14)	C16—C15—H15	120.9
C5—C4—H4	120.1	C14—C15—H15	120.9
C3—C4—H4	120.1	C15—C16—C11	123.37 (13)
C4—C5—C6	120.74 (13)	C15—C16—N13	116.56 (12)
C4—C5—H5	119.6	C11—C16—N13	120.06 (12)
C6—C5—H5	119.6	O12—N11—O13	123.34 (12)
C7—C6—C5	120.45 (14)	O12—N11—C12	119.68 (12)
C7—C6—H6	119.8	O13—N11—C12	116.99 (11)
C5—C6—H6	119.8	O14—N12—O15	124.04 (12)
C6—C7—C8	119.64 (13)	O14—N12—C14	117.92 (11)
C6—C7—H7	120.2	O15—N12—C14	118.04 (12)
C8—C7—H7	120.2	O16—N13—O17	123.57 (12)
C7—C8—C3	120.31 (12)	O16—N13—C16	118.27 (12)
C7—C8—C1	121.39 (12)	O17—N13—C16	118.15 (12)
C3—C8—C1	118.29 (12)	C11—O11—H11	106.6 (16)
C1—N1—N2—C2	−0.1 (2)	C11—C12—C13—C14	0.0 (2)
N2—N1—C1—O1	−177.43 (12)	N11—C12—C13—C14	−177.71 (11)
N2—N1—C1—C8	2.34 (19)	C12—C13—C14—C15	−0.7 (2)
N1—N2—C2—C3	−1.3 (2)	C12—C13—C14—N12	177.76 (12)
N2—C2—C3—C8	0.3 (2)	C13—C14—C15—C16	−0.2 (2)
N2—C2—C3—C4	−179.38 (13)	N12—C14—C15—C16	−178.67 (12)
C8—C3—C4—C5	−0.9 (2)	C14—C15—C16—C11	1.9 (2)
C2—C3—C4—C5	178.79 (13)	C14—C15—C16—N13	−178.00 (11)

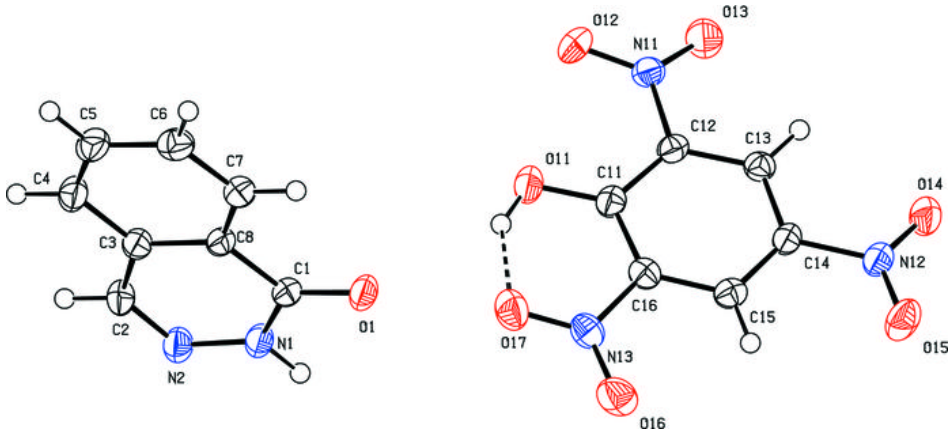
C3—C4—C5—C6	−0.1 (2)	O11—C11—C16—C15	175.42 (13)
C4—C5—C6—C7	1.0 (2)	C12—C11—C16—C15	−2.40 (19)
C5—C6—C7—C8	−0.8 (2)	O11—C11—C16—N13	−4.7 (2)
C6—C7—C8—C3	−0.22 (19)	C12—C11—C16—N13	177.46 (11)
C6—C7—C8—C1	179.16 (12)	C13—C12—N11—O12	−170.29 (12)
C4—C3—C8—C7	1.09 (19)	C11—C12—N11—O12	11.95 (19)
C2—C3—C8—C7	−178.64 (12)	C13—C12—N11—O13	9.31 (18)
C4—C3—C8—C1	−178.31 (12)	C11—C12—N11—O13	−168.45 (12)
C2—C3—C8—C1	1.96 (18)	C13—C14—N12—O14	−7.04 (19)
O1—C1—C8—C7	−2.7 (2)	C15—C14—N12—O14	171.43 (13)
N1—C1—C8—C7	177.49 (12)	C13—C14—N12—O15	173.74 (12)
O1—C1—C8—C3	176.65 (12)	C15—C14—N12—O15	−7.79 (19)
N1—C1—C8—C3	−3.12 (17)	C15—C16—N13—O16	−7.40 (18)
O11—C11—C12—C13	−176.48 (12)	C11—C16—N13—O16	172.73 (12)
C16—C11—C12—C13	1.42 (18)	C15—C16—N13—O17	171.79 (12)
O11—C11—C12—N11	1.12 (19)	C11—C16—N13—O17	−8.08 (18)
C16—C11—C12—N11	179.02 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.94 (2)	1.89 (2)	2.8252 (16)	175.2 (17)
O11—H11···O17	0.90 (3)	1.79 (3)	2.5819 (16)	146 (2)

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

Fig. 1


C5
C6
C7
C4
C3
C8
C1
O1
C2
N1
N2
O12
O13
N11
C12
C13
O11
C11
O14
C14
N12
C16
C15
O17
N13
O15
O16