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3-Aminobenzoic acid–4-nitrobenzoic acid (1/1)

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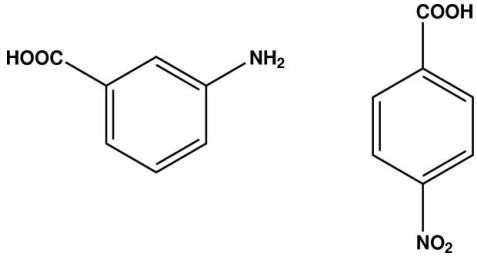
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.068; wR factor = 0.179; data-to-parameter ratio = 17.5.

In the title 1:1 adduct, $C_7H_5NO_4\cdot C_7H_7NO_2$, the nitro group of the 4-nitro benzoic acid is twisted from the attached ring by 4.40 (8)°. In the crystal, the molecules are linked into ribbon-like structures along [150] and [1$\bar{5}$0] *via* O—H···O, N—H···O, N—H···N and C—H···O intermolecular hydrogen bonds.

Related literature

For the applications of 3-aminobenzoic acid, see; Windholz (1976). For related structures, see: Bowers *et al.* (2005); Tonogaki *et al.* (1993); Voogd *et al.* (1980).



Experimental

Crystal data

$C_7H_5NO_4\cdot C_7H_7NO_2$
M_r = 304.26
Monoclinic, $C2/c$
a = 25.3707 (8) Å
b = 4.9875 (2) Å
c = 21.7276 (7) Å
β = 109.230 (2)°
V = 2595.93 (16) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 100.0 (1) K
0.24 × 0.09 × 0.06 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.971, T_{max} = 0.993
15472 measured reflections
3759 independent reflections
2197 reflections with $I > 2\sigma(I)$
R_{int} = 0.068

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.179
S = 1.01
3759 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1*O4*···O5^{i}	0.89 (4)	1.73 (4)	2.612 (2)	171 (3)
O6—H1*O6*···O3^{ii}	0.91 (4)	1.75 (4)	2.652 (2)	171 (4)
N2—H1*N1*···O2^{iii}	1.06 (4)	2.29 (4)	3.309 (3)	161 (3)
N2—H2*N2*···O2^{iv}	0.90 (3)	2.60 (3)	3.351 (3)	142 (2)
C2—H2*A*···O5^{v}	0.95	2.58	3.288 (3)	131
C4—H4*A*···O6^{iv}	0.95	2.55	3.339 (3)	141
C10—H10*A*···O1^{iii}	0.95	2.57	3.460 (3)	156

Symmetry codes: (i) $x+\frac{1}{2}, y-\frac{3}{2}, z$; (ii) $x-\frac{1}{2}, y+\frac{3}{2}, z$; (iii) $x, y-1, z$; (iv) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2714).

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supporting information

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3-Aminobenzoic acid–4-nitrobenzoic acid (1/1)

Ching Kheng Quah, Samuel Robinson Jebas and Hoong-Kun Fun

S1. Comment

3-Aminobenzoic acid is used as an intermediate for dyes, pesticides and in other organic synthesis (Windholz, 1976). The crystal structures of 3-aminobenzoic acid (Voogd *et al.*, 1980) and 4-aminobenzoic acid-4-nitrobenzoic acid have been reported (Bowers *et al.*, 2005). As a part of our investigation of the interactions between acids, we report herein the crystal structure of the title compound.

The asymmetric unit (Fig. 1) contains one 3-aminobenzoic acid molecule and one 4-nitrobenzoic acid molecule. The bond lengths and angles of 3-aminobenzoic acid and 4-nitrobenzoic acid are found to have normal values (Voogd *et al.*, 1980; Tonogaki *et al.*, 1993). Both the molecules are almost planar with the maximum deviation from planarity being 0.026 (2) Å for atom O5 of 3-aminobenzoic acid molecule, and 0.078 (2) Å for atom O1 of nitrobenzoic acid molecule. In the 4-nitrobenzoic acid molecule, the nitro group is twisted slightly from the attached ring; the dihedral angle between C1—C6 and O1—O2/C3/N1 planes is 4.40 (8)°.

The crystal packing is consolidated by O—H···O, N—H···O, N—H···N and C—H···O intermolecular hydrogen bonds (Table 1). These hydrogen bonds link the molecules into ribbon like structures along [1 5 0] and [1 $\bar{5}$ 0] (Fig.2).

S2. Experimental

3-Aminobenzoic acid and 4-nitrobenzoic acid were mixed in methanol (20 ml) in a 1:1 molar ratio. The clear colourless solution obtained was allowed to evaporate slowly. Colourless crystals were obtained after 2 d.

S3. Refinement

N and O-bound H atoms were located in a difference Fourier map and were allowed to refine freely. All the other H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

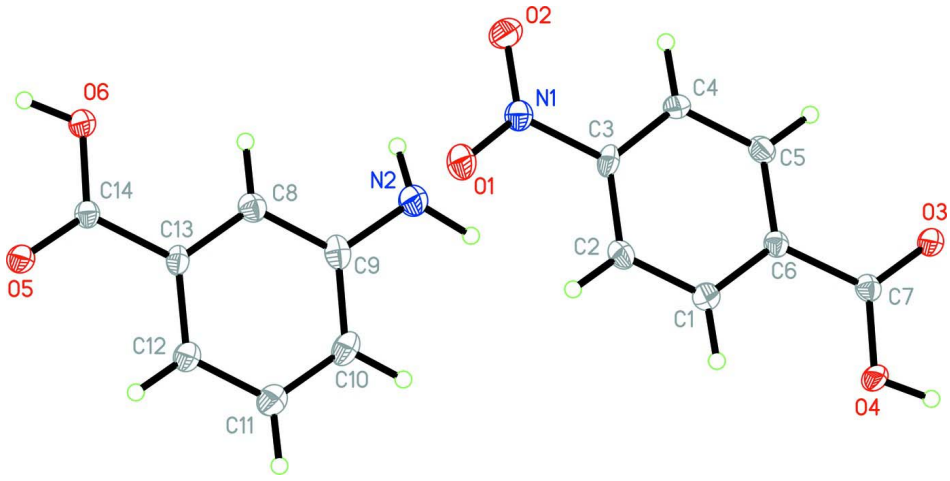

Figure 1

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

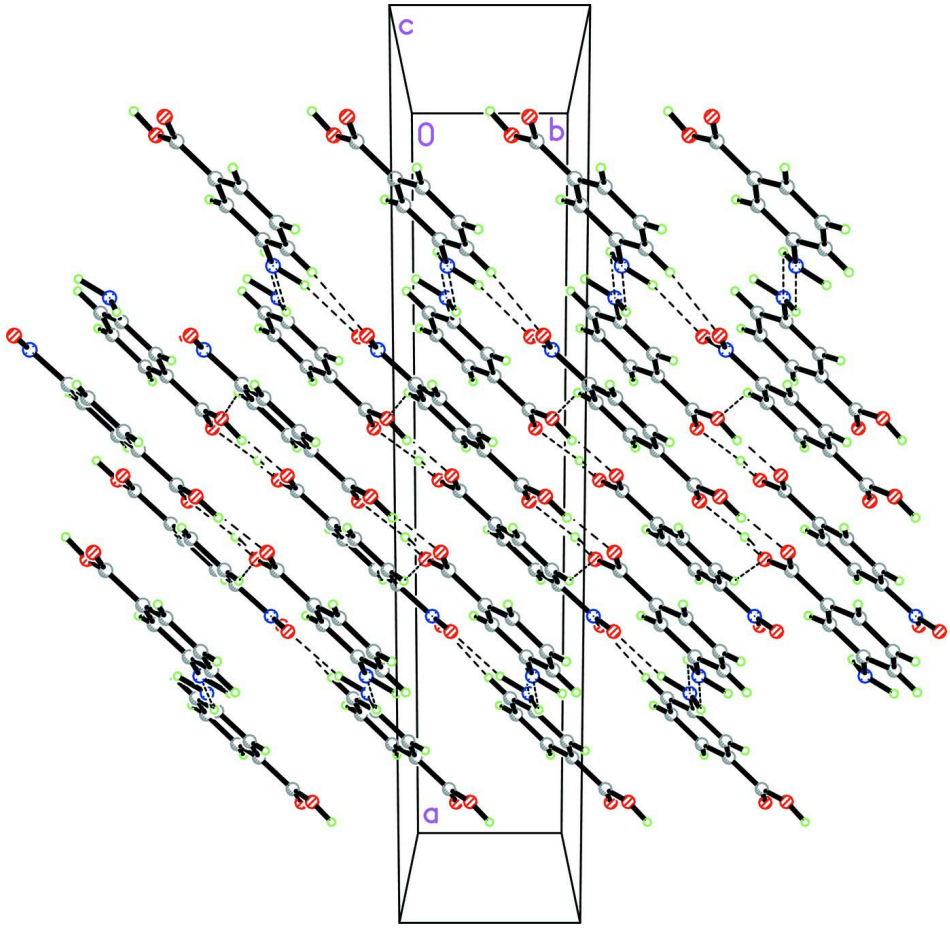

Figure 2

The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

3-Aminobenzoic acid–4-nitrobenzoic acid (1/1)

Crystal data

$C_7H_5NO_4 \cdot C_7H_7NO_2$
$M_r = 304.26$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 25.3707$ (8) Å
$b = 4.9875$ (2) Å
$c = 21.7276$ (7) Å
$\beta = 109.230$ (2)°
$V = 2595.93$ (16) Å^3
$Z = 8$
$F(000) = 1264$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2404 reflections
$\theta = 3.0$–$29.9°$
$\mu = 0.12$ mm^{-1}
$T = 100$ K
Plate, yellow
0.24 × 0.09 × 0.06 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.971$, $T_{max} = 0.993$
15472 measured reflections
3759 independent reflections
2197 reflections with $I > 2\sigma(I)$
$R_{int} = 0.068$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -34 \rightarrow 35$
$k = -7 \rightarrow 7$
$l = -29 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.179$
$S = 1.01$
3759 reflections
215 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2 + 1.6119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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}
O1	0.82025 (7)	0.6966 (4)	0.14306 (8)	0.0238 (4)
O2	0.81699 (7)	0.7604 (3)	0.04310 (8)	0.0236 (4)

O3	1.01559 (7)	−0.2306 (3)	0.07932 (8)	0.0175 (4)
O4	1.01017 (7)	−0.3174 (3)	0.17847 (8)	0.0183 (4)
O5	0.57710 (6)	0.7825 (3)	0.18023 (8)	0.0180 (4)
O6	0.58739 (7)	0.8769 (4)	0.08408 (8)	0.0194 (4)
N1	0.83479 (8)	0.6430 (4)	0.09588 (9)	0.0178 (4)
N2	0.73488 (9)	0.2432 (5)	0.06366 (11)	0.0217 (5)
C1	0.93325 (9)	0.0854 (5)	0.16778 (11)	0.0166 (5)
H1A	0.9461	−0.0152	0.2070	0.020*
C2	0.89370 (9)	0.2853 (5)	0.16067 (11)	0.0167 (5)
H2A	0.8792	0.3241	0.1948	0.020*
C3	0.87598 (9)	0.4267 (5)	0.10277 (11)	0.0158 (5)
C4	0.89605 (9)	0.3786 (5)	0.05146 (11)	0.0160 (5)
H4A	0.8831	0.4800	0.0123	0.019*
C5	0.93576 (9)	0.1775 (5)	0.05923 (11)	0.0164 (5)
H5A	0.9503	0.1395	0.0251	0.020*
C6	0.95413 (8)	0.0322 (5)	0.11703 (10)	0.0136 (5)
C7	0.99642 (9)	−0.1847 (4)	0.12311 (11)	0.0145 (5)
C8	0.66801 (9)	0.4869 (5)	0.10050 (11)	0.0172 (5)
H8A	0.6584	0.5966	0.0627	0.021*
C9	0.70819 (9)	0.2837 (5)	0.10949 (11)	0.0179 (5)
C10	0.72180 (10)	0.1297 (5)	0.16603 (12)	0.0199 (5)
H10A	0.7492	−0.0069	0.1728	0.024*
C11	0.69646 (9)	0.1707 (5)	0.21230 (12)	0.0203 (5)
H11A	0.7066	0.0630	0.2505	0.024*
C12	0.65613 (9)	0.3688 (5)	0.20347 (11)	0.0180 (5)
H12A	0.6383	0.3962	0.2351	0.022*
C13	0.64223 (9)	0.5267 (5)	0.14746 (11)	0.0152 (5)
C14	0.59973 (9)	0.7398 (4)	0.13881 (11)	0.0143 (5)
H1O4	1.0354 (14)	−0.442 (8)	0.1783 (15)	0.056 (11)*
H1O6	0.5600 (15)	0.998 (8)	0.0809 (16)	0.063 (11)*
H1N1	0.7575 (14)	0.064 (8)	0.0643 (16)	0.063 (11)*
H2N2	0.7158 (12)	0.302 (6)	0.0233 (14)	0.029 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0264 (9)	0.0247 (10)	0.0238 (10)	0.0060 (7)	0.0131 (8)	−0.0027 (7)
O2	0.0266 (9)	0.0214 (10)	0.0227 (9)	0.0058 (7)	0.0079 (7)	0.0042 (7)
O3	0.0198 (8)	0.0161 (9)	0.0190 (8)	0.0049 (7)	0.0095 (7)	0.0019 (7)
O4	0.0226 (9)	0.0164 (9)	0.0182 (9)	0.0086 (7)	0.0098 (7)	0.0039 (7)
O5	0.0213 (8)	0.0155 (9)	0.0190 (9)	0.0037 (7)	0.0090 (7)	0.0012 (7)
O6	0.0222 (9)	0.0206 (9)	0.0185 (9)	0.0069 (7)	0.0108 (7)	0.0035 (7)
N1	0.0180 (9)	0.0171 (10)	0.0187 (10)	0.0008 (8)	0.0067 (8)	−0.0014 (8)
N2	0.0229 (11)	0.0244 (12)	0.0197 (11)	0.0051 (9)	0.0096 (9)	0.0015 (9)
C1	0.0168 (11)	0.0159 (12)	0.0173 (12)	0.0005 (9)	0.0060 (9)	0.0008 (9)
C2	0.0180 (11)	0.0171 (12)	0.0173 (12)	−0.0008 (9)	0.0091 (9)	−0.0019 (9)
C3	0.0123 (10)	0.0125 (12)	0.0227 (12)	0.0023 (8)	0.0057 (9)	−0.0028 (9)
C4	0.0180 (11)	0.0138 (11)	0.0173 (12)	0.0020 (9)	0.0073 (9)	0.0034 (9)

C5	0.0181 (11)	0.0164 (12)	0.0168 (12)	0.0000 (9)	0.0087 (9)	0.0002 (9)
C6	0.0121 (10)	0.0125 (11)	0.0164 (11)	−0.0018 (8)	0.0051 (8)	−0.0007 (9)
C7	0.0139 (10)	0.0132 (12)	0.0169 (12)	−0.0018 (9)	0.0058 (9)	−0.0010 (9)
C8	0.0174 (11)	0.0155 (12)	0.0195 (12)	−0.0017 (9)	0.0073 (9)	−0.0011 (9)
C9	0.0151 (11)	0.0173 (12)	0.0222 (12)	−0.0025 (9)	0.0075 (9)	−0.0058 (9)
C10	0.0172 (11)	0.0151 (12)	0.0251 (13)	0.0029 (9)	0.0040 (10)	−0.0019 (10)
C11	0.0193 (12)	0.0179 (13)	0.0224 (13)	0.0012 (9)	0.0052 (10)	0.0006 (9)
C12	0.0184 (11)	0.0163 (12)	0.0197 (12)	0.0025 (9)	0.0069 (9)	0.0000 (9)
C13	0.0126 (10)	0.0138 (11)	0.0201 (12)	0.0010 (9)	0.0066 (9)	−0.0014 (9)
C14	0.0140 (10)	0.0137 (11)	0.0155 (11)	0.0000 (9)	0.0053 (8)	−0.0014 (9)

Geometric parameters (Å, º)

O1—N1	1.228 (2)	C3—C4	1.391 (3)
O2—N1	1.233 (2)	C4—C5	1.392 (3)
O3—C7	1.225 (3)	C4—H4A	0.95
O4—C7	1.315 (3)	C5—C6	1.391 (3)
O4—H1O4	0.89 (4)	C5—H5A	0.95
O5—C14	1.235 (3)	C6—C7	1.498 (3)
O6—C14	1.317 (3)	C8—C13	1.396 (3)
O6—H1O6	0.91 (4)	C8—C9	1.405 (3)
N1—C3	1.475 (3)	C8—H8A	0.95
N2—C9	1.391 (3)	C9—C10	1.392 (3)
N2—H1N1	1.06 (4)	C10—C11	1.375 (3)
N2—H2N2	0.90 (3)	C10—H10A	0.95
C1—C2	1.387 (3)	C11—C12	1.390 (3)
C1—C6	1.397 (3)	C11—H11A	0.95
C1—H1A	0.95	C12—C13	1.394 (3)
C2—C3	1.382 (3)	C12—H12A	0.95
C2—H2A	0.95	C13—C14	1.481 (3)
C7—O4—H1O4	109 (2)	C1—C6—C7	120.9 (2)
C14—O6—H1O6	111 (2)	O3—C7—O4	124.3 (2)
O1—N1—O2	123.7 (2)	O3—C7—C6	121.5 (2)
O1—N1—C3	118.17 (19)	O4—C7—C6	114.23 (19)
O2—N1—C3	118.17 (18)	C13—C8—C9	119.6 (2)
C9—N2—H1N1	120.1 (18)	C13—C8—H8A	120.2
C9—N2—H2N2	114.7 (18)	C9—C8—H8A	120.2
H1N1—N2—H2N2	114 (3)	N2—C9—C10	120.9 (2)
C2—C1—C6	119.8 (2)	N2—C9—C8	120.5 (2)
C2—C1—H1A	120.1	C10—C9—C8	118.6 (2)
C6—C1—H1A	120.1	C11—C10—C9	121.5 (2)
C3—C2—C1	118.3 (2)	C11—C10—H10A	119.2
C3—C2—H2A	120.8	C9—C10—H10A	119.2
C1—C2—H2A	120.8	C10—C11—C12	120.3 (2)
C2—C3—C4	123.1 (2)	C10—C11—H11A	119.8
C2—C3—N1	118.23 (19)	C12—C11—H11A	119.8
C4—C3—N1	118.6 (2)	C11—C12—C13	119.0 (2)

C3—C4—C5	117.9 (2)	C11—C12—H12A	120.5
C3—C4—H4A	121.0	C13—C12—H12A	120.5
C5—C4—H4A	121.0	C12—C13—C8	120.9 (2)
C6—C5—C4	119.9 (2)	C12—C13—C14	118.7 (2)
C6—C5—H5A	120.0	C8—C13—C14	120.4 (2)
C4—C5—H5A	120.0	O5—C14—O6	122.6 (2)
C5—C6—C1	120.8 (2)	O5—C14—C13	121.7 (2)
C5—C6—C7	118.24 (19)	O6—C14—C13	115.72 (19)
C6—C1—C2—C3	0.1 (3)	C5—C6—C7—O4	−178.0 (2)
C1—C2—C3—C4	−0.3 (3)	C1—C6—C7—O4	1.3 (3)
C1—C2—C3—N1	−178.7 (2)	C13—C8—C9—N2	−179.2 (2)
O1—N1—C3—C2	3.6 (3)	C13—C8—C9—C10	−1.0 (3)
O2—N1—C3—C2	−176.6 (2)	N2—C9—C10—C11	178.8 (2)
O1—N1—C3—C4	−175.0 (2)	C8—C9—C10—C11	0.7 (3)
O2—N1—C3—C4	4.9 (3)	C9—C10—C11—C12	0.1 (4)
C2—C3—C4—C5	0.2 (3)	C10—C11—C12—C13	−0.7 (3)
N1—C3—C4—C5	178.7 (2)	C11—C12—C13—C8	0.3 (3)
C3—C4—C5—C6	−0.1 (3)	C11—C12—C13—C14	−179.2 (2)
C4—C5—C6—C1	0.0 (3)	C9—C8—C13—C12	0.5 (3)
C4—C5—C6—C7	179.3 (2)	C9—C8—C13—C14	−179.9 (2)
C2—C1—C6—C5	0.0 (3)	C12—C13—C14—O5	1.0 (3)
C2—C1—C6—C7	−179.3 (2)	C8—C13—C14—O5	−178.6 (2)
C5—C6—C7—O3	1.7 (3)	C12—C13—C14—O6	−178.2 (2)
C1—C6—C7—O3	−179.0 (2)	C8—C13—C14—O6	2.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1*O*4···O5^{i}	0.89 (4)	1.73 (4)	2.612 (2)	171 (3)
O6—H1*O*6···O3^{ii}	0.91 (4)	1.75 (4)	2.652 (2)	171 (4)
N2—H1*N*1···O2^{iii}	1.06 (4)	2.29 (4)	3.309 (3)	161 (3)
N2—H2*N*2···O2^{iv}	0.90 (3)	2.60 (3)	3.351 (3)	142 (2)
C2—H2*A*···O5^{v}	0.95	2.58	3.288 (3)	131
C4—H4*A*···O6^{iv}	0.95	2.55	3.339 (3)	141
C10—H10*A*···O1^{iii}	0.95	2.57	3.460 (3)	156

Symmetry codes: (i) *x*+1/2, *y*−3/2, *z*; (ii) *x*−1/2, *y*+3/2, *z*; (iii) *x*, *y*−1, *z*; (iv) −*x*+3/2, −*y*+3/2, −*z*; (v) −*x*+3/2, *y*−1/2, −*z*+1/2.