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Hydrogen-bonding patterns in 2-amino-4,6-dimethoxypyrimidine–4-aminobenzoic acid (1/1)

Kaliyaperumal Thanigaimani,[a] Packianathan Thomas Muthiah[a]* and Daniel E. Lynch[b]

[a]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India, and [b]Faculty of Health and Life Sciences, Coventry University, Priory Street, Coventry CV1 5FB, England

Correspondence e-mail: tommtrichy@yahoo.co.in

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Key indicators

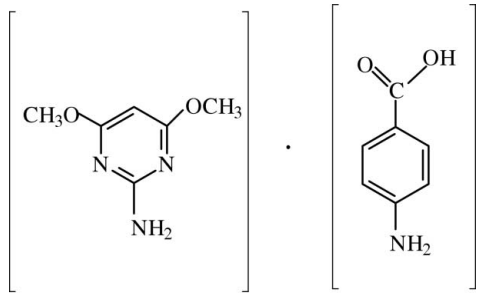
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.127
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title cocrystal, $C_6H_9N_3O_2{\cdot}C_7H_7NO_2$, the 2-amino-4,6-dimethoxypyrimidine molecule interacts with the carboxyl group of the 4-aminobenzoic acid molecule through N—H···O and O—H···N hydrogen bonds, forming a cyclic hydrogen-bonded motif [$R_2^2(8)$]. This motif further self-organizes through N—H···O hydrogen bonds to generate an array of six hydrogen bonds with the rings having the graph-set notation $R_2^3(6)$, $R_2^2(8)$, $R_4^2(8)$, $R_2^2(8)$ and $R_2^3(6)$. The 4-aminobenzoic acid molecules self-assemble *via* N—H···O hydrogen bonds to form a supramolecular chain along the *c* axis.

Comment

Pyrimidine and aminopyrimidine derivatives are biologically important compounds as they occur in nature as components of nucleic acids. Some aminopyrimidine derivatives are used as antifolate drugs (Hunt *et al.*, 1980; Baker & Santi, 1965). The adducts of carboxylic acids with 2-aminoheterocylic ring systems form a graph-set motif of $R_2^2(8)$ (Lynch & Jones, 2004). The crystal structure of 2-amino-4,6-dimethoxy pyrimidine has also been reported (Low *et al.*, 2002). The crystal structure of 4-aminobenzoic acid (Lai & Marsh, 1967) is known. The interplay of strong N—H···O and O—H···N hydrogen bonds, and weak C—H···O interactions, forms supramolecular motifs, involved in the molecular packing of organic solids. (Taylor & Kennard, 1982). In the present study, the hydrogen-bonding patterns in the 2-amino-4,6-dimethoxypyrimidine–4-aminobenzoic acid (1/1) cocrystal, (I), are investigated.



(I)

The asymmetric unit (Fig. 1) contains one 2-amino-4,6-dimethoxypyrimidine molecule and one 4-aminobenzoic acid molecule, which are linked by N2—H2*B*···O3 and O4—H4···N1 hydrogen bonds (Table 1), forming an eight-membered ring of graph-set notation $R_2^2(8)$ (Etter, 1990; Bernstein *et al.*, 1995). This type of pairing has been observed in the crystal structure of 2-aminopyrimidine–fumaric acid (Goswami *et al.*, 1999) and 2-aminopyrimidine–(+)-camphoric

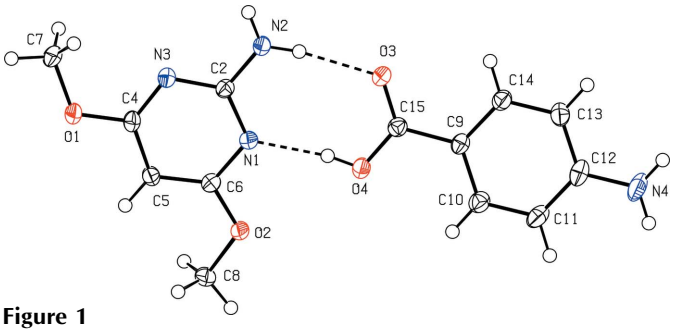


Figure 1
A view of the asymmetric unit of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

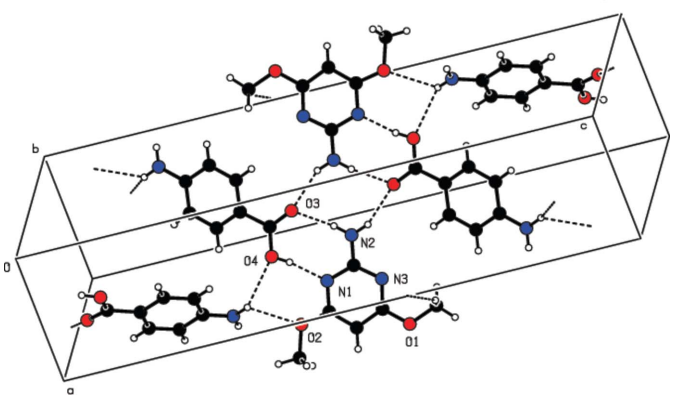


Figure 2
Hydrogen-bonding (dashed lines) patterns in compound (I).

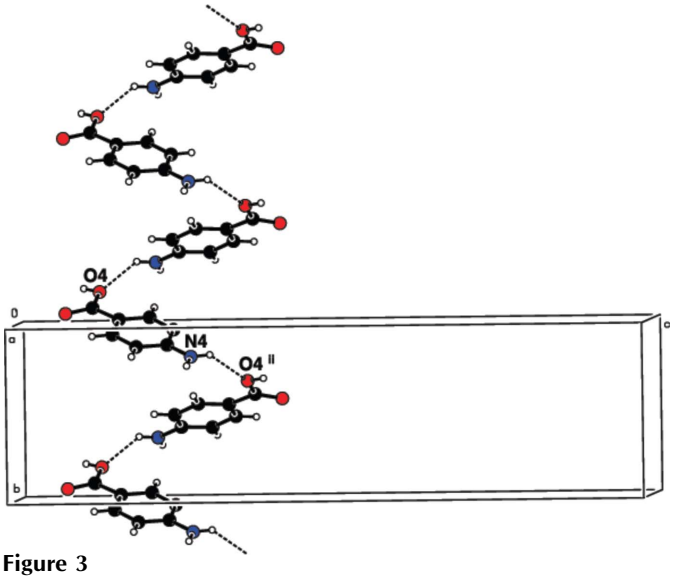


Figure 3
Hydrogen-bonding (dashed lines) patterns in the supramolecular chain in compound (I) [symmetry code: (ii) $1-x, \frac{1}{2}+y, \frac{1}{2}-z$].

acid (Goswami *et al.*, 2000). This motif further self organizes through N—H···O hydrogen bonds (Fig. 2) to generate an array of six hydrogen bonds with the rings having the graph-set notations $R_2^3(6)$, $R_2^2(8)$, $R_4^2(8)$, $R_2^2(8)$ and $R_2^3(6)$. The 4-aminobenzoic acid molecules self-assemble *via* N—H···O hydrogen bonds to form a supramolecular chain along the *c* axis, with the graph-set notation $C(9)$; this is shown in Fig. 3. The pyrimidine ring is centrosymmetrically linked through a pair of C—H···O hydrogen bonds involving a methyl group (C7) and methoxy atom O2. A π–π stacking interaction between two aminopyrimidine groups (at x, y, z and $-x, 1-y, -z$), with a perpendicular separation of 3.306 Å, a centroid–centroid distance of 3.4129 (8) Å and a slip angle (the angle between the centroid vector and the normal to the plane) of 14.39° has also been observed. These are typical aromatic stacking values (Hunter, 1994).

Experimental

A hot methanol solution (20 ml) of 2-amino-4,6-dimethoxy pyrimidine (38 mg, Aldrich) and 4-aminobenzoic acid (34 mg, Loba Chemie) was warmed for half an hour over a water bath. The mixture was cooled slowly and kept at room temperature; after a few days, colourless plate-like crystals were obtained.

Crystal data

$C_6H_9N_3O_2\cdot C_7H_7NO_2$
$M_r = 292.30$
Monoclinic, $P2_1/c$
$a = 6.6358$ (4) Å
$b = 7.5560$ (5) Å
$c = 27.4226$ (16) Å
$\beta = 94.418$ (2)°
$V = 1370.89$ (15) Å^3
$Z = 4$
$D_x = 1.416$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Plate, colourless
0.44 × 0.32 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: none
14577 measured reflections
3130 independent reflections
2469 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.127$
$S = 1.03$
3130 reflections
194 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.4081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.016 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.86	2.07	2.8546 (17)	152
N2—H2B···O3	0.86	1.96	2.8180 (17)	172
O4—H4···N1	0.82	1.83	2.6426 (16)	171
N4—H4A···O2^{ii}	0.86	2.47	3.0621 (18)	127
N4—H4A···O4^{ii}	0.86	2.45	3.1566 (18)	140
C7—H7C···O2^{iii}	0.96	2.60	3.4578 (18)	150

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

All H atoms were positioned geometrically and were refined using a riding model. The C—H, O—H and N—H bond lengths are 0.93–0.96, 0.82 and 0.86 Å, respectively [U_{iso}(H) = 1.2U_{eq}(parent atom)].

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

ORTEPII (Johnson, 1976); software used to prepare material for publication: *PLATON* (Spek, 2003).

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supporting information

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Crystal data

$C_6H_9N_3O_2·C_7H_7NO_2$
M_r = 292.30
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.6358 (4) Å
b = 7.5560 (5) Å
c = 27.4226 (16) Å
β = 94.418 (2)°
V = 1370.89 (15) Å^3
Z = 4
$F(000)$ = 616
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 50 reflections
θ = 3.5–27.5°
μ = 0.11 mm^{-1}
T = 293 K
Block, colourless
0.44 × 0.32 × 0.08 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
φ and ω scans
14577 measured reflections
3130 independent reflections
2469 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 27.5°, θ_{min} = 3.5°
h = −8→8
k = −9→9
l = −35→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.03
3130 reflections
194 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
$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.4081P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Extinction correction: SHELXL97, FC*=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.016 (4)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
O1	−0.31949 (15)	0.65274 (14)	−0.06558 (4)	0.0243 (3)
O2	−0.10312 (15)	0.62294 (13)	0.10295 (4)	0.0217 (3)
N1	0.08267 (17)	0.75316 (15)	0.04909 (4)	0.0191 (3)
N2	0.29134 (19)	0.87629 (17)	−0.00431 (5)	0.0253 (4)
N3	−0.01324 (18)	0.76844 (16)	−0.03678 (4)	0.0195 (3)
C2	0.1169 (2)	0.79880 (18)	0.00271 (5)	0.0189 (4)
C4	−0.1827 (2)	0.68686 (18)	−0.02791 (5)	0.0193 (4)
C5	−0.2328 (2)	0.62919 (19)	0.01814 (5)	0.0201 (4)
C6	−0.0914 (2)	0.66662 (18)	0.05589 (5)	0.0187 (4)
C7	−0.2659 (2)	0.7008 (2)	−0.11380 (5)	0.0253 (4)
C8	−0.2692 (2)	0.5117 (2)	0.11441 (5)	0.0235 (4)
O3	0.54244 (16)	0.93414 (15)	0.08183 (4)	0.0259 (3)
O4	0.31653 (16)	0.82162 (15)	0.12926 (4)	0.0255 (3)
N4	0.9479 (2)	1.1681 (2)	0.28970 (5)	0.0359 (5)
C9	0.6046 (2)	0.96732 (18)	0.16731 (5)	0.0199 (4)
C10	0.5327 (2)	0.9594 (2)	0.21373 (5)	0.0250 (4)
C11	0.6456 (3)	1.0262 (2)	0.25418 (5)	0.0285 (5)
C12	0.8345 (2)	1.10420 (19)	0.24943 (6)	0.0255 (4)
C13	0.9069 (2)	1.1109 (2)	0.20280 (6)	0.0254 (5)
C14	0.7943 (2)	1.04466 (19)	0.16252 (5)	0.0226 (4)
C15	0.4837 (2)	0.90465 (19)	0.12278 (5)	0.0200 (4)
H2A	0.31900	0.90570	−0.03330	0.0300*
H2B	0.37700	0.89720	0.02020	0.0300*
H5	−0.35280	0.57010	0.02280	0.0240*
H7A	−0.21140	0.81850	−0.11310	0.0300*
H7B	−0.38410	0.69650	−0.13630	0.0300*
H7C	−0.16660	0.61950	−0.12420	0.0300*
H8A	−0.39440	0.57150	0.10560	0.0280*
H8B	−0.25900	0.48660	0.14880	0.0280*
H8C	−0.26480	0.40300	0.09640	0.0280*
H4	0.25400	0.80470	0.10270	0.0310*
H4A	0.90290	1.16030	0.31820	0.0430*
H4B	1.06370	1.21580	0.28640	0.0430*
H10	0.40730	0.90870	0.21760	0.0300*
H11	0.59540	1.01910	0.28490	0.0340*

H13	1.03280	1.16090	0.19900	0.0300*
H14	0.84470	1.05130	0.13190	0.0270*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0209 (5)	0.0329 (6)	0.0182 (5)	−0.0042 (4)	−0.0035 (4)	0.0017 (4)
O2	0.0212 (5)	0.0271 (6)	0.0166 (5)	−0.0056 (4)	0.0005 (4)	0.0028 (4)
N1	0.0188 (6)	0.0212 (6)	0.0174 (6)	−0.0017 (5)	0.0016 (5)	0.0004 (5)
N2	0.0229 (7)	0.0361 (7)	0.0166 (6)	−0.0102 (5)	−0.0005 (5)	0.0010 (5)
N3	0.0189 (6)	0.0212 (6)	0.0181 (6)	−0.0003 (5)	−0.0009 (5)	−0.0004 (5)
C2	0.0206 (7)	0.0192 (7)	0.0169 (7)	−0.0004 (5)	0.0012 (5)	−0.0014 (5)
C4	0.0186 (7)	0.0192 (7)	0.0193 (7)	0.0019 (5)	−0.0031 (5)	−0.0013 (5)
C5	0.0173 (7)	0.0223 (7)	0.0204 (7)	−0.0028 (5)	−0.0004 (6)	0.0009 (5)
C6	0.0211 (7)	0.0174 (6)	0.0176 (7)	0.0009 (5)	0.0015 (5)	0.0003 (5)
C7	0.0250 (8)	0.0337 (8)	0.0167 (7)	0.0009 (7)	−0.0023 (6)	0.0022 (6)
C8	0.0218 (7)	0.0266 (8)	0.0224 (7)	−0.0048 (6)	0.0033 (6)	0.0037 (6)
O3	0.0248 (6)	0.0361 (6)	0.0167 (5)	−0.0060 (5)	0.0010 (4)	−0.0019 (4)
O4	0.0250 (6)	0.0331 (6)	0.0181 (5)	−0.0088 (5)	−0.0012 (4)	0.0003 (4)
N4	0.0475 (9)	0.0392 (8)	0.0192 (7)	−0.0113 (7)	−0.0092 (6)	−0.0018 (6)
C9	0.0237 (7)	0.0184 (7)	0.0173 (7)	0.0000 (6)	−0.0011 (6)	0.0006 (5)
C10	0.0295 (8)	0.0246 (7)	0.0207 (7)	−0.0039 (6)	0.0014 (6)	0.0010 (6)
C11	0.0402 (9)	0.0287 (8)	0.0165 (7)	−0.0044 (7)	0.0012 (7)	−0.0001 (6)
C12	0.0345 (9)	0.0189 (7)	0.0215 (7)	0.0007 (6)	−0.0075 (6)	−0.0003 (6)
C13	0.0238 (8)	0.0264 (8)	0.0252 (8)	−0.0032 (6)	−0.0031 (6)	−0.0001 (6)
C14	0.0244 (8)	0.0253 (8)	0.0178 (7)	0.0008 (6)	0.0000 (6)	0.0001 (6)
C15	0.0206 (7)	0.0205 (7)	0.0188 (7)	0.0015 (6)	0.0011 (6)	0.0004 (5)

Geometric parameters (Å, º)

O1—C4	1.3465 (17)	C5—H5	0.9303
O1—C7	1.4420 (18)	C7—H7A	0.9597
O2—C6	1.3401 (17)	C7—H7C	0.9601
O2—C8	1.4399 (17)	C7—H7B	0.9604
O3—C15	1.2370 (17)	C8—H8C	0.9600
O4—C15	1.2985 (17)	C8—H8B	0.9592
O4—H4	0.8200	C8—H8A	0.9601
N1—C2	1.3538 (18)	C9—C15	1.4860 (19)
N1—C6	1.3527 (18)	C9—C10	1.3947 (19)
N2—C2	1.3244 (18)	C9—C14	1.4032 (19)
N3—C4	1.3213 (18)	C10—C11	1.385 (2)
N3—C2	1.3517 (18)	C11—C12	1.400 (2)
N2—H2B	0.8608	C12—C13	1.401 (2)
N2—H2A	0.8588	C13—C14	1.379 (2)
N4—C12	1.375 (2)	C10—H10	0.9296
N4—H4A	0.8599	C11—H11	0.9310
N4—H4B	0.8598	C13—H13	0.9300
C4—C5	1.3999 (19)	C14—H14	0.9288

C5—C6	1.3720 (19)		
O1···C8^{i}	3.1974 (17)	C8···H7C^{v}	3.0493
O2···N4^{ii}	3.0621 (18)	C8···H5	2.5688
O2···O4	3.1968 (15)	C8···H7B^{i}	2.8881
O3···C6^{iii}	3.2806 (17)	C9···H7B^{vi}	3.0207
O3···N2^{iv}	2.8546 (17)	C11···H10^{vii}	3.0194
O3···N2	2.8180 (17)	C12···H10^{vii}	2.9848
O3···C5^{iii}	3.3144 (18)	C13···H4B^{ix}	3.0049
O4···N1	2.6426 (16)	C14···H4B^{ix}	2.9701
O4···N4^{ii}	3.1566 (18)	C15···H2B	2.8479
O4···O2	3.1968 (15)	C15···H8A^{iii}	2.6966
O1···H8C^{i}	2.8535	C15···H7A^{vi}	2.7636
O1···H8A^{i}	2.7127	H2A···O3^{iv}	2.0663
O2···H4	2.7394	H2A···H2B^{iv}	2.5109
O2···H7C^{v}	2.5958	H2B···H2A^{iv}	2.5109
O2···H4A^{ii}	2.4653	H2B···H2B^{iv}	2.5660
O3···H14	2.5035	H2B···O3	1.9631
O3···H8A^{iii}	2.8402	H2B···C15	2.8479
O3···H2B	1.9631	H2B···H4	2.5608
O3···H2A^{iv}	2.0663	H2B···N2^{iv}	2.8479
O4···H10	2.5376	H4···O2	2.7394
O4···H7A^{vi}	2.8337	H4···N1	1.8298
O4···H4A^{ii}	2.4505	H4···C6	2.7452
O4···H8A^{iii}	2.8043	H4···H2B	2.5608
N1···O4	2.6426 (16)	H4···C2	2.8220
N1···C15	3.4128 (18)	H4A···O4^{vii}	2.4505
N1···C4^{v}	3.4484 (18)	H4A···H11	2.4184
N2···O3	2.8180 (17)	H4A···O2^{vii}	2.4653
N2···O3^{iv}	2.8546 (17)	H4B···C13^{x}	3.0049
N3···C6^{v}	3.4087 (18)	H4B···C14^{x}	2.9701
N3···C5^{v}	3.4388 (19)	H4B···H13	2.4254
N4···O4^{vii}	3.1566 (18)	H5···H8C	2.4139
N4···O2^{vii}	3.0621 (18)	H5···H5^{i}	2.4751
N1···H4	1.8298	H5···C8	2.5688
N2···H2B^{iv}	2.8479	H5···H8A	2.3083
N3···H7C	2.7701	H7A···O4^{vi}	2.8337
N3···H7A	2.4142	H7A···N3	2.4142
N3···H8C^{v}	2.8670	H7A···C15^{vi}	2.7636
N4···H8B^{vii}	2.9070	H7B···C9^{vi}	3.0207
C2···C5^{v}	3.383 (2)	H7B···C8^{i}	2.8881
C2···C2^{vi}	3.4115 (19)	H7C···O2^{v}	2.5958
C4···N1^{v}	3.4484 (18)	H7C···C8^{v}	3.0493
C4···C6^{v}	3.3535 (19)	H7C···N3	2.7701
C5···C2^{v}	3.383 (2)	H8A···O3^{viii}	2.8402
C5···N3^{v}	3.4388 (19)	H8A···C5	2.7365
C5···O3^{viii}	3.3144 (18)	H8A···C15^{viii}	2.6966
C6···N3^{v}	3.4087 (18)	H8A···O4^{viii}	2.8043

C6···C4^{v}	3.3535 (19)	H8A···C7^{i}	3.0730
C6···O3^{viii}	3.2806 (17)	H8A···O1^{i}	2.7127
C7···C15^{vi}	3.314 (2)	H8A···H5	2.3083
C7···C8^{i}	3.477 (2)	H8B···N4^{ii}	2.9070
C8···O1^{i}	3.1974 (17)	H8C···C5	2.7644
C8···C7^{i}	3.477 (2)	H8C···N3^{v}	2.8670
C8···C15^{viii}	3.408 (2)	H8C···H5	2.4139
C15···C8^{iii}	3.408 (2)	H8C···O1^{i}	2.8535
C15···N1	3.4128 (18)	H10···O4	2.5376
C15···C7^{vi}	3.314 (2)	H10···C11^{ii}	3.0194
C2···H4	2.8220	H10···C12^{ii}	2.9848
C5···H8C	2.7644	H11···H4A	2.4184
C5···H8A	2.7365	H13···H4B	2.4254
C6···H4	2.7452	H13···C7^{iv}	3.0822
C7···H13^{iv}	3.0822	H14···O3	2.5035
C7···H8A^{i}	3.0730		

C4—O1—C7	117.13 (11)	H7B—C7—H7C	109.43
C6—O2—C8	117.14 (11)	O2—C8—H8B	109.44
C15—O4—H4	109.45	O2—C8—H8C	109.45
C2—N1—C6	117.36 (11)	H8A—C8—H8B	109.55
C2—N3—C4	115.59 (12)	O2—C8—H8A	109.41
C2—N2—H2A	120.03	H8A—C8—H8C	109.46
C2—N2—H2B	119.97	H8B—C8—H8C	109.51
H2A—N2—H2B	120.00	C14—C9—C15	119.16 (12)
H4A—N4—H4B	120.01	C10—C9—C14	118.41 (12)
C12—N4—H4B	120.06	C10—C9—C15	122.37 (12)
C12—N4—H4A	119.93	C9—C10—C11	120.89 (13)
N1—C2—N3	124.50 (12)	C10—C11—C12	120.78 (14)
N1—C2—N2	117.45 (12)	N4—C12—C11	120.76 (14)
N2—C2—N3	118.05 (13)	N4—C12—C13	121.02 (13)
O1—C4—C5	116.07 (12)	C11—C12—C13	118.19 (14)
O1—C4—N3	118.76 (12)	C12—C13—C14	121.01 (13)
N3—C4—C5	125.16 (12)	C9—C14—C13	120.72 (13)
C4—C5—C6	114.86 (12)	O3—C15—C9	120.05 (12)
O2—C6—C5	126.07 (12)	O4—C15—C9	117.02 (12)
N1—C6—C5	122.50 (12)	O3—C15—O4	122.93 (13)
O2—C6—N1	111.43 (11)	C9—C10—H10	119.61
C6—C5—H5	122.56	C11—C10—H10	119.50
C4—C5—H5	122.59	C10—C11—H11	119.64
O1—C7—H7B	109.49	C12—C11—H11	119.58
O1—C7—H7C	109.55	C12—C13—H13	119.41
O1—C7—H7A	109.52	C14—C13—H13	119.58
H7A—C7—H7B	109.39	C9—C14—H14	119.69
H7A—C7—H7C	109.43	C13—C14—H14	119.60

C7—O1—C4—N3	2.95 (18)	C4—C5—C6—N1	0.2 (2)
C7—O1—C4—C5	−176.20 (12)	C10—C9—C14—C13	0.1 (2)

C8—O2—C6—N1	−172.72 (11)	C15—C9—C10—C11	−177.09 (14)
C8—O2—C6—C5	6.5 (2)	C14—C9—C10—C11	0.0 (2)
C2—N1—C6—C5	−1.8 (2)	C10—C9—C15—O4	−8.2 (2)
C6—N1—C2—N2	−176.98 (12)	C15—C9—C14—C13	177.30 (13)
C6—N1—C2—N3	2.0 (2)	C10—C9—C15—O3	171.01 (14)
C2—N1—C6—O2	177.50 (11)	C14—C9—C15—O3	−6.1 (2)
C2—N3—C4—O1	179.85 (12)	C14—C9—C15—O4	174.77 (13)
C4—N3—C2—N2	178.36 (13)	C9—C10—C11—C12	0.3 (2)
C4—N3—C2—N1	−0.7 (2)	C10—C11—C12—N4	−179.01 (14)
C2—N3—C4—C5	−1.1 (2)	C10—C11—C12—C13	−0.7 (2)
N3—C4—C5—C6	1.3 (2)	N4—C12—C13—C14	179.12 (14)
O1—C4—C5—C6	−179.61 (12)	C11—C12—C13—C14	0.8 (2)
C4—C5—C6—O2	−178.93 (13)	C12—C13—C14—C9	−0.5 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3^{iv}	0.86	2.07	2.8546 (17)	152
N2—H2*B*···O3	0.86	1.96	2.8180 (17)	172
O4—H4···N1	0.82	1.83	2.6426 (16)	171
N4—H4*A*···O2^{vii}	0.86	2.47	3.0621 (18)	127
N4—H4*A*···O4^{vii}	0.86	2.45	3.1566 (18)	140
C7—H7*C*···O2^{v}	0.96	2.60	3.4578 (18)	150

Symmetry codes: (iv) −*x*+1, −*y*+2, −*z*; (v) −*x*, −*y*+1, −*z*; (vii) −*x*+1, *y*+1/2, −*z*+1/2.