Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hydrogen-bonding patterns in the cocrystal 2,4-diamino-6-phenyl-1,3,5-triazine–sorbic acid (1/1)

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

[a]School of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, Tamilnadu, India, and [b]Faculty of Health and Life Sciences, Coventry University, Priory Street, Coventry CV1 5FB, England
Correspondence e-mail: tommtrichy@yahoo.co.in

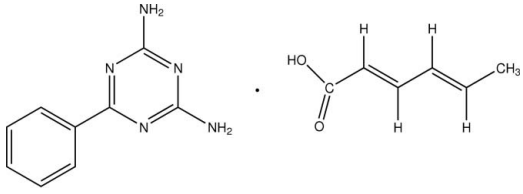
Received 22 October 2007; accepted 23 October 2007

Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.059; wR factor = 0.150; data-to-parameter ratio = 17.3.

In the title cocrystal, $C_9H_9N_5\cdot C_6H_8O_2$, the asymmetric unit contains one 2,4-diamino-6-phenyl-1,3,5-triazine molecule and a sorbic acid molecule. The triazine molecules are base-paired [with a graph set of $R_2^2(8)$] on either side *via* N—H···N hydrogen bonds, forming a supramolecular ribbon along the *c* axis. Each triazine molecule interacts with the carboxyl group of a sorbic acid molecule *via* N—H···O and O—H···N hydrogen bonds, generating $R_2^2(8)$ motifs. The supramolecular ribbons are interlinked by N—H···O hydrogen bonds involving the 2-amino group of the triazine molecules and the carboxyl O atom of the sorbic acid molecule.

Related literature

For related literature, see: Bernstein *et al.* (1995); Bork *et al.* (2003); Chen *et al.* (2001); Cox (1994); Desiraju (1989); Diaz-Ortiz *et al.* (2004); Etter (1990); Habibi *et al.* (2007); Janczak & Perpétuo (2004); Lynch & Jones (2004); MacDonald & Whitesides (1994); Martindale (1996); Raj *et al.* (2003); Sheshmani *et al.* (2006); Perpétuo & Janczak (2007).



Experimental

Crystal data

$C_9H_9N_5\cdot C_6H_8O_2$
M_r = 299.34
Monoclinic, $C2/c$
a = 33.867 (2) Å
b = 7.4289 (3) Å
c = 12.2015 (8) Å
β = 94.241 (2)°
V = 3061.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.44 × 0.34 × 0.22 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Absorption correction: none
15418 measured reflections
3490 independent reflections
2409 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.151
S = 1.10
3490 reflections
202 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N3	0.82	1.82	2.6337 (18)	171
N2—H2A···O1^{i}	0.86	2.35	2.9477 (19)	127
N2—H2B···N5^{ii}	0.86	2.22	3.0771 (19)	179
N4—H4A···O1	0.86	2.04	2.8935 (19)	169
N4—H4B···N1^{iii}	0.86	2.18	3.031 (2)	169
C12—H12···N1	0.93	2.45	2.775 (3)	101

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) 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: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

KT thanks UGC (New Delhi) for the UGC-Rajiv Gandhi Junior Research Fellowship [Reference No. F.16–12/2000 (SA-II)]. DL thanks the EPSRC National Crystallography Service (Southampton, England) for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2556).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bork, J. T., Lee, J. W., Khersonsky, S. M., Moon, H. S. & Chang, Y. T. (2003). *Org. Lett.* **5**, 117–120.
Chen, W.-Q., Weng, L.-H. & Jin, G.-Y. (2001). *Acta Cryst.* E**57**, o91–o93.
Cox, P. J. (1994). *Acta Cryst.* C**50**, 1620–1622.
Desiraju, G. R. (1989). *Crystal Engineering: The Design of Organic Solids*. Amsterdam: Elsevier.
Diaz-Ortiz, A., Elguero, J., Foces-Foces, C., de la Hoz, A., Moreno, A., del Carmen Mateo, M., Sanchez-Migallon, A. & Valiente, G. (2004). *New J. Chem.* **28**, 952–958.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Habibi, M. H., Zendehdel, M., Barati, K., Harrington, R. W. & Clegg, W. (2007). *Acta Cryst.* C**63**, o474–o476.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Janczak, J. & Perpétuo, G. J. (2004). *Acta Cryst.* C**60**, o211–o214.
Lynch, D. E. & Jones, G. D. (2004). *Acta Cryst.* B**60**, 748–754.
MacDonald, J. C. & Whitesides, G. M. (1994). *Chem. Rev.* **94**, 2383–2420.
Martindale, W. (1996). *The Extra Pharmacopoeia*, 30th ed. London: Pharmaceutical Press.

  doi:10.1107/S1600536807052543

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*. Vol. 276, *Macromolecular Crystallography*, part A. edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Perpétuo, G. J. & Janczak, J. (2007). *Acta Cryst.* C**63**, o271–o273.
Raj, S. B., Stanley, N., Muthiah, P. T., Bocelli, G., Olla, R. & Cantoni, A. (2003). *Cryst. Growth Des.* **3**, 567–571.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheshmani, S., Ghadermazi, M., Aghabozorg, H. & Nakhjavan, B. (2006). *Acta Cryst.* E**62**, o4681–o4682.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2007). E**63**, o4450-o4451 [**doi:10.1107/S1600536807052543**]

Hydrogen-bonding patterns in the cocrystal 2,4-diamino-6-phenyl-1,3,5-triazine-sorbic acid (1/1)

K. Thanigaimani, P. T. Muthiah and D. E. Lynch

Comment

Hydrogen bonding plays a key role in molecular recognition, crystal engineering and supramolecular chemistry (Desiraju, 1989). Heterocycles play an important role in the study of pharmaceuticals and agrochemicals. Many derivatives of nitrogen heterocyclic rings such as triazine have been synthesized in recent years (Chen *et al.*, 2001). Triazine derivatives show antitumor activity as well as broad range of biological activities like anti-angiogenesis and antimicrobial effects (Bork *et al.*, 2003). The organic and inorganic complexes of triazine form well defined non-covalent supramolecular architectures *via* multiple hydrogen bonds constituting arrays of hydrogen-bonding sites (MacDonald & Whitesides, 1994). The adducts of carboxylic acids with 2-aminoheterocylic ring system forms a graph-set motif of $R_2^2(8)$ (Lynch & Jones, 2004). The crystal structure of 2,4-diamino-6-phenyl-1,3,5-triazine (Diaz-Ortiz *et al.*, 2004), Melaminium maleate monohydrate (Janczak *et al.*, 2004), 2,4-diamino-6-methyl-1,3,5-triazin-1-ium trifluoroacetate (Perpétuo & Janczak, 2007), 4-(dimethylamino)-benzaldehyde and 6-phenyl-1,3,5-triazine- 2,4-diamine (Habibi *et al.*, 2007) and 2,6-diamino-4-phenyltriazinium chloride monohydrate (Sheshmani *et al.*, 2006) have also been reported in the literature. The crystal structure of sorbic acid (Cox, 1994) is known. Sorbic acid is an antibacterial agent and widely used as a preservative (Martindale, 1996). The sorbic acid moiety lies in the EE configuration. The extended conformation of the sorbic acid can be inferred from the four torsion angles (C13—C14—C15—C16) 179.26 (16)°, (C14—C15—C16—C17) 178.28 (18)°, (C15—C16—C17—C18) −179.48 (18)° and (O1—C13—C14—C15) 177.82 (17)°. This conformation is similar to the trimethoprim sorbate dihydrate (Raj *et al.*, 2003). In the present study, the hydrogen-bonding patterns in the 2,4-diamino-6- phenyl-1,3,5-triazine sorbic acid (1/1) cocrystal, (I), are investigated.

The asymmetric unit (Fig. 1) contains one 2,4-diamino-6-phenyl-1,3,5- triazine molecule and one sorbic acid molecule. The triazine molecules are base paired [with a graph-set of $R_2^2(8)$] on either sides *via* N—H···N hydrogen bonds forming a supramolecular ribbon along the *c* axis (Fig. 2). Each triazine molecule interacts with the carboxyl group of a sorbic acid molecule *via* N—H···O and O—H···N hydrogen bonds, generating $R_2^2(8)$ motifs (Etter, 1990; Bernstein *et al.*, 1995). The supramolecular ribbons are interlinked by N—H···O hydrogen bonds involving 2-amino group of the triazine molecules and carboxyl oxygen of the sorbic acid molecules.

Experimental

A hot methanol solution (20 ml) of 2,4-diamino-6-phenyl-1,3,5-triazine (31 mg A ldrich) and sorbic acid (28 mg Loba) 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.

Refinement

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

Figures

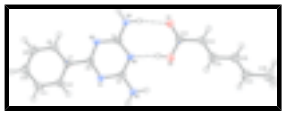


Fig. 1. The asymmetric unit of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

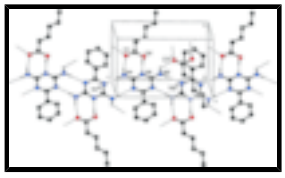


Fig. 2. The crystal structure of (III). Dashed lines indicate hydrogen bonds [symmetry code: (i) *x*, −*y* + 1, *z* − 1/2; (ii) *x*, −*y*, *z* − 1/2; (iii) *x*, −*y*, *z* + 1/2]

2,4-diamino-6-phenyl-1,3,5-triazine–sorbic acid (1/1)

Crystal data

$C_9H_9N_5·C_6H_8O_2$	F_{000} = 1264
M_r = 299.34	D_x = 1.299 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 25 reflections
a = 33.867 (2) Å	θ = 3.3–27.5º
b = 7.4289 (3) Å	μ = 0.09 mm^{-1}
c = 12.2015 (8) Å	*T* = 120 K
β = 94.241 (2)º	Plate, colourless
V = 3061.4 (3) Å^3	0.44 × 0.34 × 0.22 mm
Z = 8	

Data collection

Bruker–Nonius 95mm CCD camera on κ-goniostat diffractometer	3490 independent reflections
Radiation source: Bruker–Nonius FR591 rotating anode	2409 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
Detector resolution: 9.091 pixels mm^{-1}	θ_{max} = 27.5º
T = 120 K	θ_{min} = 3.3º
φ and ω scans	*h* = −42→44
Absorption correction: none	*k* = −7→9
15418 measured reflections	*l* = −15→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.059	$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2 + 1.012P]$ where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.151$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.10$	$\Delta\rho_{max} = 0.46$ e Å^{-3}
3490 reflections	$\Delta\rho_{min} = -0.47$ e Å^{-3}
202 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0114 (10)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.33830 (4)	−0.02806 (18)	0.59344 (11)	0.0218 (4)
N2	0.36560 (5)	0.21597 (18)	0.51237 (11)	0.0272 (5)
N3	0.36902 (4)	0.20752 (17)	0.70125 (11)	0.0215 (4)
N4	0.36933 (5)	0.19093 (19)	0.88889 (11)	0.0278 (5)
N5	0.34027 (4)	−0.04358 (18)	0.78884 (11)	0.0217 (4)
C2	0.35752 (5)	0.1316 (2)	0.60467 (13)	0.0211 (5)
C4	0.35938 (5)	0.1172 (2)	0.79131 (13)	0.0213 (5)
C6	0.33086 (5)	−0.1085 (2)	0.68777 (13)	0.0196 (5)
C7	0.30998 (5)	−0.2847 (2)	0.67783 (13)	0.0218 (5)
C8	0.30691 (5)	−0.3975 (2)	0.76805 (14)	0.0265 (5)
C9	0.28704 (6)	−0.5603 (2)	0.75629 (16)	0.0316 (6)
C10	0.26997 (6)	−0.6115 (3)	0.65530 (17)	0.0412 (7)
C11	0.27256 (8)	−0.5011 (3)	0.56587 (18)	0.0543 (8)
C12	0.29259 (6)	−0.3383 (3)	0.57683 (15)	0.0404 (7)
O1	0.40728 (4)	0.53754 (16)	0.87083 (10)	0.0306 (4)
O2	0.40583 (4)	0.51815 (16)	0.68782 (10)	0.0334 (4)
C13	0.41368 (5)	0.6024 (2)	0.78110 (14)	0.0247 (5)
C14	0.43088 (5)	0.7830 (2)	0.77198 (15)	0.0279 (6)
C15	0.43979 (5)	0.8600 (2)	0.67794 (15)	0.0259 (5)
C16	0.45628 (5)	1.0387 (2)	0.67058 (16)	0.0289 (6)
C17	0.46605 (6)	1.1137 (2)	0.57754 (16)	0.0333 (6)
C18	0.48345 (7)	1.2975 (3)	0.56732 (19)	0.0429 (7)
H2A	0.37800	0.31710	0.51570	0.0330*
H2B	0.35840	0.16920	0.44960	0.0330*

H4A	0.38150	0.29260	0.89280	0.0330*
H4B	0.36360	0.13680	0.94800	0.0330*
H8	0.31830	−0.36340	0.83660	0.0320*
H9	0.28520	−0.63500	0.81690	0.0380*
H10	0.25670	−0.72080	0.64760	0.0490*
H11	0.26090	−0.53560	0.49770	0.0650*
H12	0.29430	−0.26450	0.51580	0.0480*
H2	0.39530	0.42140	0.69930	0.0500*
H14	0.43590	0.84850	0.83640	0.0330*
H15	0.43510	0.79460	0.61330	0.0310*
H16	0.46030	1.10520	0.73500	0.0350*
H17	0.46170	1.04640	0.51350	0.0400*
H18A	0.48580	1.35430	0.63820	0.0640*
H18B	0.46650	1.36840	0.51760	0.0640*
H18C	0.50920	1.28770	0.53960	0.0640*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0282 (8)	0.0219 (7)	0.0154 (7)	−0.0008 (6)	0.0032 (6)	−0.0006 (5)
N2	0.0455 (10)	0.0219 (8)	0.0142 (7)	−0.0042 (6)	0.0027 (7)	0.0004 (5)
N3	0.0313 (8)	0.0214 (7)	0.0121 (7)	−0.0007 (6)	0.0031 (6)	−0.0007 (5)
N4	0.0466 (10)	0.0237 (8)	0.0133 (7)	−0.0073 (6)	0.0031 (6)	−0.0003 (6)
N5	0.0280 (8)	0.0231 (8)	0.0142 (7)	−0.0007 (6)	0.0022 (6)	−0.0014 (5)
C2	0.0268 (9)	0.0195 (8)	0.0172 (8)	0.0038 (6)	0.0023 (7)	0.0007 (6)
C4	0.0257 (9)	0.0225 (9)	0.0160 (8)	0.0021 (7)	0.0029 (7)	0.0007 (6)
C6	0.0210 (8)	0.0226 (9)	0.0153 (8)	0.0037 (6)	0.0027 (7)	−0.0002 (6)
C7	0.0228 (9)	0.0245 (9)	0.0188 (8)	0.0000 (7)	0.0053 (7)	−0.0028 (7)
C8	0.0301 (10)	0.0273 (9)	0.0222 (9)	−0.0009 (7)	0.0019 (8)	−0.0006 (7)
C9	0.0360 (11)	0.0267 (10)	0.0331 (11)	−0.0024 (8)	0.0096 (8)	0.0014 (8)
C10	0.0521 (14)	0.0370 (11)	0.0366 (12)	−0.0214 (9)	0.0178 (10)	−0.0122 (9)
C11	0.0776 (17)	0.0617 (15)	0.0241 (11)	−0.0389 (13)	0.0079 (11)	−0.0139 (10)
C12	0.0558 (14)	0.0462 (12)	0.0196 (10)	−0.0238 (10)	0.0059 (9)	−0.0027 (8)
O1	0.0455 (8)	0.0263 (7)	0.0203 (7)	−0.0054 (5)	0.0054 (6)	−0.0022 (5)
O2	0.0508 (9)	0.0287 (7)	0.0217 (7)	−0.0119 (6)	0.0088 (6)	−0.0052 (5)
C13	0.0291 (10)	0.0250 (9)	0.0203 (9)	0.0011 (7)	0.0033 (7)	−0.0024 (7)
C14	0.0322 (10)	0.0269 (9)	0.0245 (10)	−0.0028 (7)	0.0013 (8)	−0.0045 (7)
C15	0.0240 (9)	0.0286 (9)	0.0249 (9)	0.0006 (7)	0.0003 (7)	−0.0009 (7)
C16	0.0262 (10)	0.0307 (10)	0.0295 (10)	−0.0018 (7)	−0.0004 (8)	0.0004 (8)
C17	0.0346 (11)	0.0332 (10)	0.0321 (11)	0.0003 (8)	0.0018 (8)	0.0072 (8)
C18	0.0452 (13)	0.0351 (12)	0.0489 (13)	−0.0036 (9)	0.0073 (10)	0.0109 (10)

Geometric parameters (Å, °)

O1—C13	1.230 (2)	C10—C11	1.373 (3)
O2—C13	1.309 (2)	C11—C12	1.388 (3)
O2—H2	0.8190	C8—H8	0.9300
N1—C6	1.337 (2)	C9—H9	0.9304
N1—C2	1.355 (2)	C10—H10	0.9294

N2—C2	1.335 (2)	C11—H11	0.9300
N3—C4	1.348 (2)	C12—H12	0.9300
N3—C2	1.338 (2)	C13—C14	1.470 (2)
N4—C4	1.331 (2)	C14—C15	1.336 (2)
N5—C4	1.358 (2)	C15—C16	1.446 (2)
N5—C6	1.340 (2)	C16—C17	1.328 (3)
N2—H2A	0.8602	C17—C18	1.496 (3)
N2—H2B	0.8597	C14—H14	0.9294
N4—H4A	0.8601	C15—H15	0.9299
N4—H4B	0.8604	C16—H16	0.9298
C6—C7	1.488 (2)	C17—H17	0.9302
C7—C8	1.393 (2)	C18—H18A	0.9603
C7—C12	1.384 (2)	C18—H18B	0.9610
C8—C9	1.386 (2)	C18—H18C	0.9612
C9—C10	1.375 (3)		
O1···N2^{i}	2.9477 (19)	C4···H2	2.8371
O1···N4	2.8935 (19)	C4···H2B^{vii}	2.8753
O2···N3	2.6337 (18)	C8···H10^{viii}	2.7841
O1···H4A	2.0445	C13···H4A	2.9260
O1···H18B^{ii}	2.6808	C16···H16^{xi}	3.0119
O1···H2A^{i}	2.3523	C17···H17^{xii}	3.0063
O2···H2A	2.6901	C17···H14^{xiii}	3.0552
O2···H15	2.4820	H2···N2	2.8642
N1···N4^{iii}	3.031 (2)	H2···N3	1.8222
N2···O1^{iv}	2.9477 (19)	H2···C4	2.8371
N2···N5^{iii}	3.0771 (19)	H2···H2A	2.4017
N3···C13	3.409 (2)	H2···C2	2.7179
N3···C16^{v}	3.257 (2)	H2A···O1^{iv}	2.3523
N3···C9^{vi}	3.378 (2)	H2A···H2	2.4017
N3···O2	2.6337 (18)	H2A···O2	2.6901
N4···O1	2.8935 (19)	H2B···N4^{iii}	2.8078
N4···N1^{vii}	3.031 (2)	H2B···N5^{iii}	2.2175
N5···C14^{v}	3.348 (2)	H2B···C4^{iii}	2.8753
N5···N2^{vii}	3.0771 (19)	H2B···H4B^{iii}	2.2803
N1···H4B^{iii}	2.1819	H2B···H8^{iii}	2.3558
N1···H12	2.4484	H4A···C13	2.9260
N2···H2	2.8642	H4A···O1	2.0445
N2···H4B^{iii}	2.7353	H4B···N1^{vii}	2.1819
N2···H8^{iii}	2.8031	H4B···H2B^{vii}	2.2802
N3···H2	1.8222	H4B···N2^{vii}	2.7353
N4···H2B^{vii}	2.8078	H4B···C2^{vii}	2.7804
N5···H8	2.5695	H8···H2B^{vii}	2.3558
N5···H2B^{vii}	2.2175	H8···N5	2.5695
C2···C16^{v}	3.451 (2)	H8···N2^{vii}	2.8031

C2···C15^{v}	3.502 (2)	H9···H12^{xiv}	2.5360
C4···C14^{v}	3.488 (2)	H10···H11^{xv}	2.5724
C4···C9^{vi}	3.431 (2)	H10···C8^{ix}	2.7841
C6···C14^{v}	3.559 (2)	H11···H10^{xv}	2.5724
C8···C10^{viii}	3.540 (3)	H12···N1	2.4484
C9···N3^{v}	3.378 (2)	H12···H9^{xvi}	2.5360
C9···C4^{v}	3.431 (2)	H14···H16	2.4498
C10···C8^{ix}	3.540 (3)	H14···C17^{ii}	3.0552
C12···C12^{x}	3.572 (3)	H14···H17^{ii}	2.4007
C13···N3	3.409 (2)	H15···O2	2.4820
C14···C4^{vi}	3.488 (2)	H15···H17	2.4404
C14···N5^{vi}	3.348 (2)	H16···H14	2.4498
C14···C6^{vi}	3.559 (2)	H16···H18A	2.3909
C15···C2^{vi}	3.502 (2)	H16···C16^{xi}	3.0119
C16···C16^{xi}	3.417 (3)	H17···H15	2.4404
C16···N3^{vi}	3.257 (2)	H17···C17^{xii}	3.0063
C16···C2^{vi}	3.451 (2)	H17···H14^{xiii}	2.4007
C17···C17^{xii}	3.517 (3)	H18A···H16	2.3909
C2···H4B^{iii}	2.7804	H18B···O1^{xiii}	2.6808
C2···H2	2.7179		
C13—O2—H2	109.51	C10—C9—H9	119.92
C2—N1—C6	115.08 (13)	C8—C9—H9	119.91
C2—N3—C4	115.84 (13)	C11—C10—H10	120.02
C4—N5—C6	114.67 (13)	C9—C10—H10	120.01
C2—N2—H2B	119.97	C10—C11—H11	119.89
H2A—N2—H2B	120.02	C12—C11—H11	119.89
C2—N2—H2A	120.01	C7—C12—H12	119.71
C4—N4—H4A	119.97	C11—C12—H12	119.69
H4A—N4—H4B	120.05	O1—C13—C14	121.45 (15)
C4—N4—H4B	119.97	O2—C13—C14	115.26 (15)
N1—C2—N3	124.36 (14)	O1—C13—O2	123.29 (14)
N1—C2—N2	116.91 (14)	C13—C14—C15	124.85 (16)
N2—C2—N3	118.73 (14)	C14—C15—C16	124.00 (16)
N3—C4—N4	117.63 (14)	C15—C16—C17	124.06 (17)
N3—C4—N5	124.30 (14)	C16—C17—C18	125.36 (17)
N4—C4—N5	118.07 (14)	C13—C14—H14	117.55
N5—C6—C7	118.07 (14)	C15—C14—H14	117.60
N1—C6—N5	125.73 (14)	C14—C15—H15	117.99
N1—C6—C7	116.20 (14)	C16—C15—H15	118.01
C6—C7—C8	121.82 (14)	C15—C16—H16	117.94
C6—C7—C12	119.59 (15)	C17—C16—H16	118.00
C8—C7—C12	118.59 (16)	C16—C17—H17	117.29
C7—C8—C9	120.46 (16)	C18—C17—H17	117.35
C8—C9—C10	120.17 (17)	C17—C18—H18A	109.45
C9—C10—C11	120.0 (2)	C17—C18—H18B	109.41

C10—C11—C12	120.2 (2)	C17—C18—H18C	109.48
C7—C12—C11	120.59 (18)	H18A—C18—H18B	109.48
C7—C8—H8	119.77	H18A—C18—H18C	109.47
C9—C8—H8	119.78	H18B—C18—H18C	109.54
C2—N1—C6—N5	0.9 (2)	N5—C6—C7—C8	−12.5 (2)
C2—N1—C6—C7	−179.65 (14)	C6—C7—C12—C11	−179.24 (19)
C6—N1—C2—N2	179.82 (15)	C12—C7—C8—C9	0.4 (3)
C6—N1—C2—N3	0.5 (2)	C6—C7—C8—C9	179.57 (16)
C2—N3—C4—N4	−178.16 (15)	C8—C7—C12—C11	0.0 (3)
C4—N3—C2—N1	−1.8 (2)	C7—C8—C9—C10	−0.3 (3)
C4—N3—C2—N2	178.90 (15)	C8—C9—C10—C11	−0.1 (3)
C2—N3—C4—N5	1.9 (2)	C9—C10—C11—C12	0.4 (3)
C4—N5—C6—N1	−0.8 (2)	C10—C11—C12—C7	−0.4 (3)
C4—N5—C6—C7	179.76 (14)	O2—C13—C14—C15	−2.3 (3)
C6—N5—C4—N4	179.35 (15)	O1—C13—C14—C15	177.82 (17)
C6—N5—C4—N3	−0.7 (2)	C13—C14—C15—C16	179.26 (16)
N1—C6—C7—C12	−12.8 (2)	C14—C15—C16—C17	178.28 (18)
N1—C6—C7—C8	167.99 (15)	C15—C16—C17—C18	−179.48 (18)
N5—C6—C7—C12	166.65 (16)		

Symmetry codes: (i) *x*, −*y*+1, *z*+1/2; (ii) *x*, −*y*+2, *z*+1/2; (iii) *x*, −*y*, *z*−1/2; (iv) *x*, −*y*+1, *z*−1/2; (v) *x*, *y*−1, *z*; (vi) *x*, *y*+1, *z*; (vii) *x*, −*y*, *z*+1/2; (viii) −*x*+1/2, *y*+1/2, −*z*+3/2; (ix) −*x*+1/2, *y*−1/2, −*z*+3/2; (x) −*x*+1/2, −*y*−1/2, −*z*+1; (xi) −*x*+1, *y*, −*z*+3/2; (xii) −*x*+1, −*y*+2, −*z*+1; (xiii) *x*, −*y*+2, *z*−1/2; (xiv) *x*, −*y*−1, *z*+1/2; (xv) −*x*+1/2, −*y*−3/2, −*z*+1; (xvi) *x*, −*y*−1, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N3	0.82	1.82	2.6337 (18)	171
N2—H2A···O1^{iv}	0.86	2.35	2.9477 (19)	127
N2—H2B···N5^{iii}	0.86	2.22	3.0771 (19)	179
N4—H4A···O1	0.86	2.04	2.8935 (19)	169
N4—H4B···N1^{vii}	0.86	2.18	3.031 (2)	169
C12—H12···N1	0.93	2.45	2.775 (3)	101

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

Fig. 1

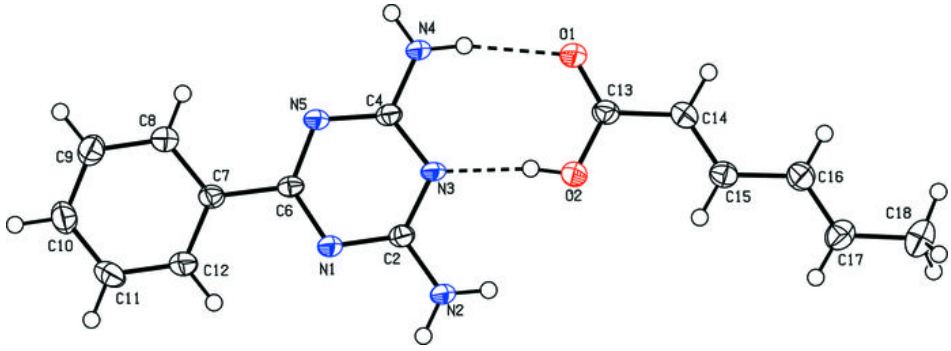

N4
O1
C13
C14
N5
C4
C8
C9
C7
N3
O2
C15
C16
C6
C10
C12
N1
C2
C18
C17
C11
N2

Fig. 2