Crystal structure and Hirshfeld surface analysis of 2-amino-4-methoxy-6-methylpyrimidinium 2-hydroxybenzoate

Muthaiah Jeevaraj,[a] Palaniyappan Sivajeyanthi,[a] Bellarmin Edison,[a] Kaliyaperumal Thanigaimani,[b] Kasthuri Balasubramani[a]* and Ibrahim Abdul Razak[c]‡

[a]Department of Chemistry, Government Arts College (Autonomous), Thanthonimalai, Karur 639 005, Tamil Nadu, India, [b]Department of Chemistry, Government Arts College, Tiruchirappalli 620 022, Tamil Nadu, India, and [c]School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia. *Correspondence e-mail: manavaibala@gmail.com

In the title molecular salt, $C_6H_{10}N_3O^+ \cdot C_7H_5O_3^-$, the cation is protonated at the N atom lying between the amine and methyl substituents and the dihedral angle between the carboxyl group and its attached ring in the anion is 4.0 (2)°. The anion features an intramolecular O—H···O hydrogen bond, which closes an $S(6)$ ring. The cation and anion are linked by two N—H···O hydrogen bonds [$R_2^2(8)$ motif] to generate an ion pair in which the dihedral angle between the aromatic rings is 8.34 (9)°. Crystal symmetry relates two ion pairs bridged by further N—H···O hydrogen bonds into a tetrameric *DDAA* array. The tetramers are linked by pairs of C—H···O hydrogen bonds to generate [100] chains. Hirshfeld surface and fingerprint plot analyses are presented.

1. chemical context

Pyrimidine and aminopyrimidine derivatives have many applications as pesticides and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely-used anti-AIDS drug (Gilchrist, 1997). Hydrogen bonding plays a vital role in molecular recognition. Supramolecular chemistry plays a pivotal role in biological systems and in artificial systems. It refers to the specific interaction between two or more motifs through non-covalent interactions such as hydrogen bonding, hydrophobic forces, van der Waals forces, π–π interactions *etc*. The generating of supramolecular architectures is correlated to the positions and properties of the active groups in molecules (Desiraju *et al.*, 1989; Steiner *et al.*, 2002) As part of our studies in these areas, the synthesis and structure of the title molecular salt, (I), is presented here.
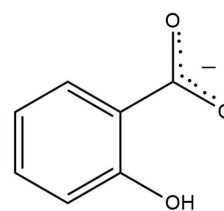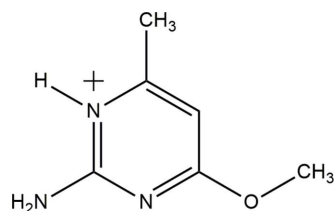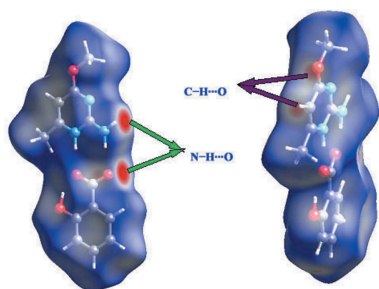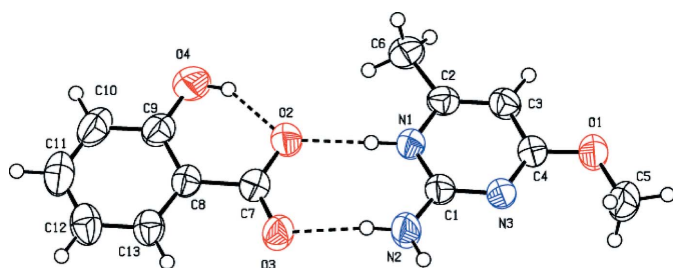
Figure 1
The asymmetric unit of (I), with 50% probability displacement ellipsoids. The hydrogen bonds are indicated by dashed lines.

2. structural commentary

The molecular structure of (I) is shown in Fig. 1. The asymmetric unit contains a 2-amino-4-methoxy-6-methylpyrimidinium cation and a 2-hydroxybenzoate anion. The cation is protonated at N1, which lies between the amine and methyl substituents: this protonation is reflected by an increase in the bond angle at N1 [C1—N1—C2 = 121.09 (15)°], when compared with the unprotonated atom N3 [C1—N3—C4 = 116.52 (18)°], and the corresponding angle of 116.01 (18)° in neutral 2-amino-4-methoxy-6-methylpyrimidine (Glidewell et al., 2003). An intramolecular O—H⋯O hydrogen bond occurs within the anion (Table 1).

3. supramolecular features

The protonated N atom (N1) and 2-amino group (N2) of the cation interacts with the O1 and O2 oxygen atoms of the carboxylate anion through a pair of N—H⋯O hydrogen bonds (Table 1), forming an eight-membered ring motif $R_2^2(8)$. Inversion-related $R_2^2(8)$ ring motifs are further bridged by N—H⋯O hydrogen bonds thereby forming a *DDAA* tetramer (*D* stands for hydrogen-bond donor and *A* stands for hydrogen-bond acceptor). This set of fused rings can be represented by the graph-set notations $R_2^2(8)$, $R_4^2(8)$ and $R_2^2(8)$. This type of motif has been reported previously in the crystal structures of trimethoprim hydrogen glutarate (Robert et al., 2001) and 2-amino-4-methoxy-6-methylpyridinium trifluoroacetate (Jeevaraj et al., 2016). These arrays are further linked *via*
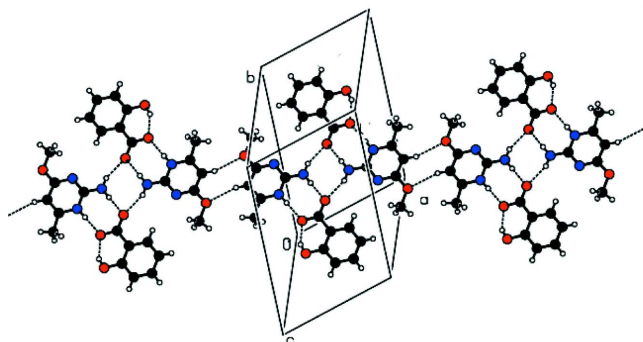
Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯O2	0.86	1.84	2.7033 (19)	176
N2—H2A⋯O3[i]	0.86	2.00	2.816 (3)	158
N2—H2B⋯O3	0.86	1.99	2.830 (2)	165
O4—H4⋯O2	0.82	1.81	2.534 (2)	147
C3—H3⋯O1[ii]	0.93	2.48	3.374 (3)	160

Symmetry codes: (i) −x + 1, −y + 1, −z + 1; (ii) −x + 3, −y + 1, −z + 2.

pairwise C—H⋯O hydrogen bonds to generate another $R_2^2(8)$ ring motif as part of a [100] chain (Fig. 2).

4. Hirshfeld surface analysis

The d_{norm} parameter takes negative or positive values depending on whether the inter-molecular contact is shorter or longer, respectively, than the van der Waals radii (Spackman & Jayatilaka et al., 2009; McKinnon et al., 2007). The d_{norm} surface of the ion-pair in (I) is shown in Fig. 3: this naturally neglects hydrogen bonds (intra-anion O—H⋯O and N—H⋯O cation-to-anion) that occur within the asymmetric unit. The red points represent closer contacts and negative d_{norm} values on the surface corresponding to the N—H⋯O and C—H⋯O interactions are light red in colour. Two-dimensional fingerprint plots from the Hirshfeld surface analysis, as shown in Fig. 4, give a break-down of different contacts as follows: H⋯H (44.2%), C⋯H/H⋯C (19.6%), O⋯H/H⋯O (20.9%), C⋯O/O⋯C (3.0%), C⋯C (2.9%), N⋯H/H⋯N (8.1%) and O⋯O (1.0%). Two 'wingtips' in the fingerprint plot are related to the strong H⋯O and O⋯H interactions.

5. Database survey

A search of the Cambridge Structural Database (Version 5.37, update February 2017; Groom et al., 2016) for 2-amino-4-
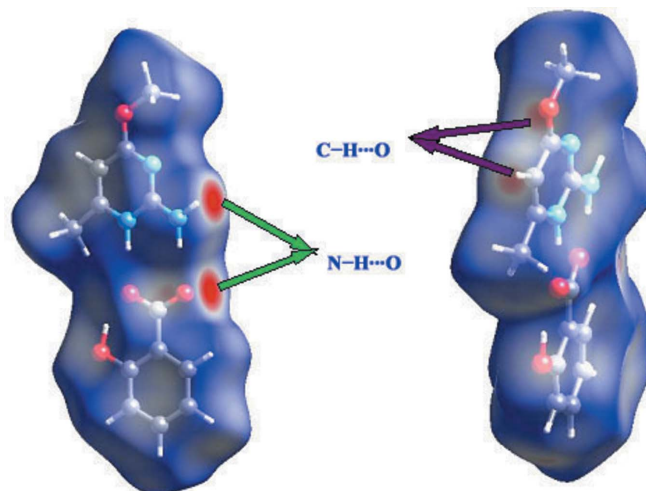

Figure 2
A [100] chain in the crystal of (I) incorporating $R_2^2(8)$, $R_4^2(8)$ and $R_4^2(12)$ ring motifs.

Figure 3
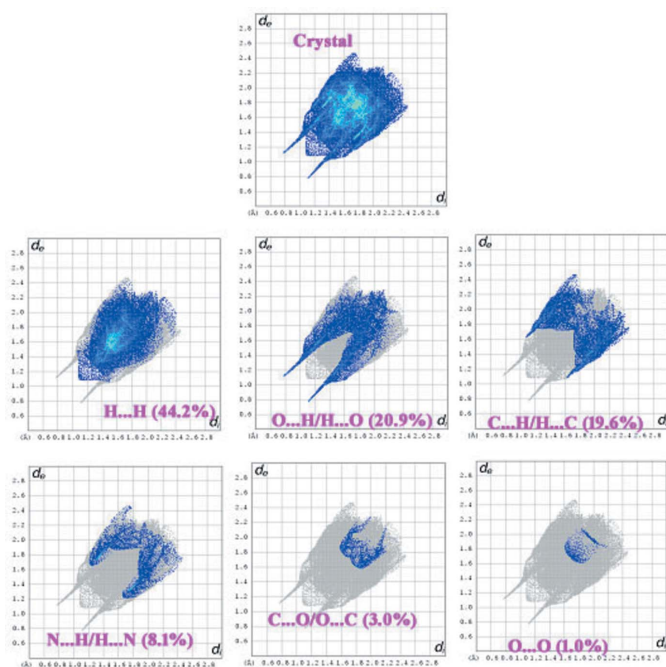Three-dimensional Hirshfeld surface of (I).

Figure 4
Fingerprint plots for (I).

methoxy-6-methylpyrimidine yielded seven structures: VAQSOW, VAQSUC, VAQSEM, VAQSIQ, VAQRUB and VAQSAI (Aakeroy *et al.*, 2003) and NUQTOJ (Jasinski *et al.* (2010).

6. Synthesis and crystallization

The title compound was synthesized by mixing hot methanolic solutions (20 ml) of 2-amino-4-methoxy-6-methylpyrimidine (0.139 mg) and 2-hydroxybenzoic acid (0.156 mg) in a 1:1 molar ratio. The mixed solutions were warmed few minutes over a waterbath and then cooled and kept at room temperature for slow evaporation. After a few days, colourless block-shaped crystals of (I) were obtained (yield = 65%).

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were positioned geometrically (N—H = 0.86, O—H = 0.82 and C—H = 0.96 or 0.93 Å) and were refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). A rotating-group model was used for the methyl group.

Funding information

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{10}N_3O^+ \cdot C_7H_5O_3^-$
M_r	277.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	9.4291 (12), 15.0620 (19), 12.1595 (11)
β (°)	128.252 (6)
V (Å^3)	1356.1 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	$0.55 \times 0.33 \times 0.16$
Data collection	
Diffractometer	Bruker KappaCCD APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.960, 0.984
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33325, 4033, 2373
R_{int}	0.042
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.708
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.056, 0.164, 1.02
No. of reflections	4033
No. of parameters	183
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.21, −0.19

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

2-Amino-4-methoxy-6-methylpyrimidinium 2-hydroxybenzoate

Crystal data

$C_6H_{10}N_3O^+\cdot C_7H_5O_3^-$	$F(000) = 584$
$M_r = 277.28$	$D_x = 1.358$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4033 reflections
$a = 9.4291$ (12) Å	$\theta = 2.5$–$27.5°$
$b = 15.0620$ (19) Å	$\mu = 0.10$ mm^{-1}
$c = 12.1595$ (11) Å	$T = 296$ K
$\beta = 128.252$ (6)°	Block, colourless
$V = 1356.1$ (3) Å^3	$0.55 \times 0.33 \times 0.16$ mm
$Z = 4$	

Data collection

Bruker KappaCCD APEXII diffractometer	33325 measured reflections
	4033 independent reflections
Radiation source: fine-focus sealed tube	2373 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.042$
ω and φ scans	$\theta_{max} = 30.2°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -13 \rightarrow 13$
	$k = -21 \rightarrow 21$
$T_{min} = 0.960$, $T_{max} = 0.984$	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.056$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.164$	
$S = 1.02$	Hydrogen site location: inferred from neighbouring sites
4033 reflections	
183 parameters	H atoms treated by a mixture of independent and constrained refinement
0 restraints	

$w = 1/[\sigma^2(F_o^2) + (0.0587P)^2 + 0.4004P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Special details

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

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 > 2sigma(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	1.29929 (16)	0.42997 (10)	1.00372 (13)	0.0632 (4)
N1	0.97381 (17)	0.55436 (9)	0.63943 (14)	0.0475 (4)
N2	0.72932 (19)	0.50804 (12)	0.62236 (17)	0.0659 (6)
N3	1.01155 (18)	0.46656 (10)	0.81604 (14)	0.0486 (4)
C1	0.9058 (2)	0.50922 (12)	0.69373 (17)	0.0482 (5)
C2	1.1545 (2)	0.55729 (11)	0.70701 (17)	0.0465 (5)
C3	1.2648 (2)	0.51464 (12)	0.82987 (18)	0.0510 (5)
C4	1.1868 (2)	0.46995 (11)	0.88151 (17)	0.0472 (5)
C5	1.2254 (3)	0.38111 (18)	1.0601 (3)	0.0863 (9)
C6	1.2148 (3)	0.60934 (14)	0.6387 (2)	0.0620 (7)
O2	0.75239 (17)	0.63571 (9)	0.38790 (13)	0.0593 (4)
O3	0.51173 (16)	0.57024 (9)	0.34276 (13)	0.0597 (4)
O4	0.7259 (2)	0.72936 (11)	0.20277 (15)	0.0756 (6)
C7	0.5836 (2)	0.62036 (11)	0.30856 (17)	0.0459 (5)
C8	0.4695 (2)	0.66507 (10)	0.16945 (16)	0.0445 (5)
C9	0.5463 (3)	0.71779 (12)	0.12434 (19)	0.0554 (6)
C10	0.4349 (4)	0.75988 (14)	−0.0047 (2)	0.0723 (8)
C11	0.2513 (3)	0.74946 (14)	−0.0879 (2)	0.0719 (8)
C12	0.1737 (3)	0.69718 (14)	−0.0458 (2)	0.0649 (7)
C13	0.2822 (2)	0.65538 (12)	0.08200 (19)	0.0529 (6)
H1	0.90150	0.58160	0.56090	0.0570*
H2A	0.68270	0.47990	0.65460	0.0790*
H2B	0.66070	0.53540	0.54350	0.0790*
H3	1.38930	0.51480	0.87920	0.0610*
H5A	1.14960	0.41960	1.06650	0.1290*
H5B	1.32220	0.35930	1.15160	0.1290*
H5C	1.15550	0.33200	0.99970	0.1290*
H6A	1.22890	0.67050	0.66590	0.0930*
H6B	1.12630	0.60460	0.53890	0.0930*
H6C	1.32820	0.58650	0.66740	0.0930*
H4	0.77590	0.70480	0.27870	0.1130*
H10	0.48530	0.79540	−0.03500	0.0870*
H11	0.17840	0.77820	−0.17400	0.0860*

H12	0.04900	0.69010	−0.10300	0.0780*
H13	0.22980	0.61990	0.11070	0.0640*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0472 (7)	0.0777 (9)	0.0528 (7)	0.0025 (6)	0.0250 (6)	0.0194 (6)
N1	0.0436 (7)	0.0531 (8)	0.0423 (7)	−0.0014 (6)	0.0249 (6)	0.0067 (6)
N2	0.0418 (8)	0.0915 (12)	0.0561 (9)	0.0001 (8)	0.0262 (7)	0.0254 (9)
N3	0.0426 (7)	0.0549 (8)	0.0442 (8)	−0.0032 (6)	0.0249 (6)	0.0054 (6)
C1	0.0433 (8)	0.0543 (10)	0.0446 (9)	−0.0026 (7)	0.0260 (8)	0.0036 (7)
C2	0.0468 (9)	0.0486 (9)	0.0478 (9)	−0.0061 (7)	0.0311 (8)	−0.0041 (7)
C3	0.0417 (8)	0.0597 (10)	0.0492 (9)	−0.0022 (7)	0.0269 (8)	0.0016 (8)
C4	0.0447 (9)	0.0496 (9)	0.0428 (9)	0.0003 (7)	0.0248 (7)	0.0021 (7)
C5	0.0666 (13)	0.1089 (19)	0.0698 (14)	−0.0019 (12)	0.0355 (12)	0.0374 (13)
C6	0.0594 (11)	0.0715 (12)	0.0613 (11)	−0.0109 (9)	0.0405 (10)	0.0042 (9)
O2	0.0508 (7)	0.0703 (8)	0.0485 (7)	−0.0047 (6)	0.0266 (6)	0.0078 (6)
O3	0.0537 (7)	0.0726 (9)	0.0564 (7)	0.0029 (6)	0.0359 (6)	0.0161 (6)
O4	0.0751 (9)	0.0866 (11)	0.0666 (9)	−0.0209 (8)	0.0446 (8)	0.0052 (8)
C7	0.0511 (9)	0.0460 (9)	0.0460 (9)	0.0039 (7)	0.0328 (8)	0.0010 (7)
C8	0.0540 (9)	0.0387 (8)	0.0421 (8)	0.0046 (7)	0.0304 (8)	0.0002 (6)
C9	0.0703 (12)	0.0485 (9)	0.0518 (10)	−0.0050 (8)	0.0400 (10)	−0.0011 (8)
C10	0.1055 (18)	0.0579 (12)	0.0625 (13)	−0.0020 (11)	0.0565 (13)	0.0097 (10)
C11	0.0920 (16)	0.0589 (12)	0.0491 (11)	0.0191 (11)	0.0359 (12)	0.0094 (9)
C12	0.0653 (12)	0.0627 (12)	0.0528 (11)	0.0186 (9)	0.0296 (10)	0.0042 (9)
C13	0.0571 (10)	0.0490 (10)	0.0502 (10)	0.0100 (8)	0.0320 (9)	0.0026 (8)

Geometric parameters (Å, º)

O1—C4	1.321 (2)	C5—H5A	0.9600
O1—C5	1.445 (4)	C5—H5C	0.9600
O2—C7	1.271 (3)	C5—H5B	0.9600
O3—C7	1.245 (3)	C6—H6B	0.9600
O4—C9	1.345 (3)	C6—H6C	0.9600
O4—H4	0.8200	C6—H6A	0.9600
N1—C2	1.359 (3)	C7—C8	1.490 (2)
N1—C1	1.354 (3)	C8—C13	1.395 (3)
N2—C1	1.317 (3)	C8—C9	1.396 (3)
N3—C1	1.335 (2)	C9—C10	1.388 (3)
N3—C4	1.318 (3)	C10—C11	1.370 (4)
N1—H1	0.8600	C11—C12	1.372 (4)
N2—H2B	0.8600	C12—C13	1.375 (3)
N2—H2A	0.8600	C10—H10	0.9300
C2—C6	1.488 (3)	C11—H11	0.9300
C2—C3	1.343 (2)	C12—H12	0.9300
C3—C4	1.400 (3)	C13—H13	0.9300
C3—H3	0.9300		

O1···C3^i	3.374 (3)	C7···H10^{iv}	2.8800
O2···C3^{ii}	3.411 (2)	C7···H2B	2.7800
O2···N1	2.7033 (19)	C7···H1	2.7100
O2···O4	2.534 (2)	C7···H4	2.4200
O3···N2^{iii}	2.816 (3)	C9···H5B^{vi}	3.0500
O3···N2	2.830 (2)	C12···H6A^{ix}	3.0300
O4···O2	2.534 (2)	C13···H6A^{ix}	2.9700
O1···H3^i	2.4800	H1···O2	1.8400
O2···H4	1.8100	H1···O3	2.9200
O2···H6B	2.8300	H1···C7	2.7100
O2···H1	1.8400	H1···H2B	2.2600
O3···H2B	1.9900	H1···H6B	2.3200
O3···H13	2.5100	H2A···O3^{iii}	2.0000
O3···H1	2.9200	H2A···H2B^{iii}	2.5800
O3···H2A^{iii}	2.0000	H2B···O3	1.9900
O3···H6C^{ii}	2.8500	H2B···C7	2.7800
O3···H10^{iv}	2.6100	H2B···H1	2.2600
O4···H12^v	2.7200	H2B···H2A^{iii}	2.5800
O4···H5B^{vi}	2.8600	H3···H6C	2.5100
N1···O2	2.7033 (19)	H3···O1^i	2.4800
N2···O3	2.830 (2)	H3···C3^i	3.0100
N2···O3^{iii}	2.816 (3)	H3···H3^i	2.3600
N3···H5C	2.6800	H4···O2	1.8100
N3···H5A	2.5600	H4···C7	2.4200
C2···C11^{vii}	3.551 (3)	H4···H12^v	2.5700
C2···C12^{vii}	3.582 (3)	H5A···N3	2.5600
C3···O1^i	3.374 (3)	H5B···O4^x	2.8600
C3···C12^{vii}	3.492 (3)	H5B···C9^x	3.0500
C3···C7^{ii}	3.463 (3)	H5C···N3	2.6800
C3···O2^{ii}	3.411 (2)	H6A···C13^v	2.9700
C4···C12^{vii}	3.556 (3)	H6A···C12^v	3.0300
C4···C13^{vii}	3.441 (3)	H6B···O2	2.8300
C6···C12^v	3.550 (3)	H6B···H1	2.3200
C7···C3^{ii}	3.463 (3)	H6C···H3	2.5100
C11···C2^{viii}	3.551 (3)	H6C···O3^{ii}	2.8500
C12···C3^{viii}	3.492 (3)	H10···O3^{xi}	2.6100
C12···C2^{viii}	3.582 (3)	H10···C7^{xi}	2.8800
C12···C4^{viii}	3.556 (3)	H12···O4^{ix}	2.7200
C12···C6^{ix}	3.550 (3)	H12···H4^{ix}	2.5700
C13···C4^{viii}	3.441 (3)	H13···O3	2.5100
C3···H3^i	3.0100		
C4—O1—C5	118.6 (2)	C2—C6—H6A	109.00
C9—O4—H4	109.00	C2—C6—H6C	109.00
C1—N1—C2	121.09 (15)	H6A—C6—H6B	109.00
C1—N3—C4	116.52 (18)	C2—C6—H6B	109.00
C1—N1—H1	119.00	H6B—C6—H6C	110.00
C2—N1—H1	119.00	H6A—C6—H6C	109.00

H2A—N2—H2B	120.00	O2—C7—C8	117.66 (18)
C1—N2—H2A	120.00	O3—C7—C8	119.57 (18)
C1—N2—H2B	120.00	O2—C7—O3	122.77 (16)
N2—C1—N3	119.68 (19)	C7—C8—C13	120.12 (18)
N1—C1—N3	122.16 (19)	C9—C8—C13	118.69 (16)
N1—C1—N2	118.17 (16)	C7—C8—C9	121.19 (19)
N1—C2—C6	116.68 (16)	O4—C9—C10	118.8 (3)
C3—C2—C6	125.0 (2)	C8—C9—C10	119.4 (3)
N1—C2—C3	118.35 (19)	O4—C9—C8	121.81 (17)
C2—C3—C4	118.0 (2)	C9—C10—C11	120.6 (3)
N3—C4—C3	123.91 (16)	C10—C11—C12	120.8 (2)
O1—C4—C3	116.42 (19)	C11—C12—C13	119.3 (2)
O1—C4—N3	119.67 (18)	C8—C13—C12	121.3 (2)
C2—C3—H3	121.00	C9—C10—H10	120.00
C4—C3—H3	121.00	C11—C10—H10	120.00
O1—C5—H5B	109.00	C10—C11—H11	120.00
O1—C5—H5C	109.00	C12—C11—H11	120.00
O1—C5—H5A	109.00	C11—C12—H12	120.00
H5A—C5—H5C	110.00	C13—C12—H12	120.00
H5B—C5—H5C	109.00	C8—C13—H13	119.00
H5A—C5—H5B	110.00	C12—C13—H13	119.00
C5—O1—C4—N3	1.9 (3)	O2—C7—C8—C13	−175.72 (17)
C5—O1—C4—C3	−178.55 (18)	O3—C7—C8—C9	−176.44 (18)
C2—N1—C1—N2	−179.22 (17)	O3—C7—C8—C13	4.1 (3)
C2—N1—C1—N3	0.8 (3)	C7—C8—C9—O4	1.2 (3)
C1—N1—C2—C3	−0.4 (2)	C7—C8—C9—C10	−178.58 (19)
C1—N1—C2—C6	−179.52 (16)	C13—C8—C9—O4	−179.40 (18)
C4—N3—C1—N1	−0.5 (3)	C13—C8—C9—C10	0.8 (3)
C4—N3—C1—N2	179.56 (17)	C7—C8—C13—C12	178.86 (18)
C1—N3—C4—O1	179.29 (16)	C9—C8—C13—C12	−0.6 (3)
C1—N3—C4—C3	−0.3 (3)	O4—C9—C10—C11	179.7 (2)
N1—C2—C3—C4	−0.3 (3)	C8—C9—C10—C11	−0.5 (3)
C6—C2—C3—C4	178.73 (18)	C9—C10—C11—C12	−0.2 (4)
C2—C3—C4—O1	−178.88 (16)	C10—C11—C12—C13	0.4 (4)
C2—C3—C4—N3	0.7 (3)	C11—C12—C13—C8	−0.1 (3)
O2—C7—C8—C9	3.7 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2	0.86	1.84	2.7033 (19)	176
N2—H2*A*···O3[iii]	0.86	2.00	2.816 (3)	158
N2—H2*B*···O3	0.86	1.99	2.830 (2)	165

O4—H4···O2	0.82	1.81	2.534 (2)	147
C3—H3···O1^i	0.93	2.48	3.374 (3)	160

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