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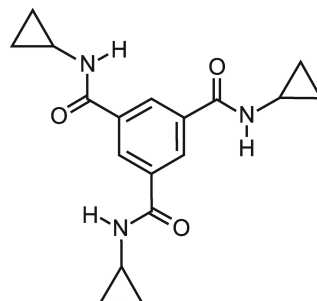
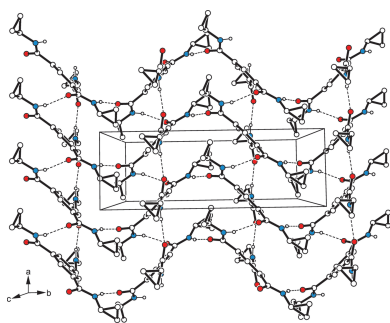
# Crystal structure of *N,N',N''*-tricyclopropylbenzene-1,3,5-tricarboxamide

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The title compound, C<sub>18</sub>H<sub>21</sub>N<sub>3</sub>O<sub>3</sub>, was prepared from 1,3,5-benzenetricarbonyl trichloride and cyclopropylamine. Its crystal structure was solved in the monoclinic space group *P*2<sub>1</sub>/*c*. In the crystal, the three amide groups of the molecule are inclined at angles of 26.5 (1), 36.9 (1) and 37.8 (1)° with respect to the plane of the benzene ring. The molecules are linked by N—H...O hydrogen bonds, forming two-dimensional supramolecular aggregates that extend parallel to the crystallographic *ab* plane and are further connected by C—H...O contacts. As a result of the supramolecular interactions, a propeller-like conformation of the title molecule can be observed.

## 1. Chemical context

The cyclopropane ring represents a building block of numerous natural products and has also been recognized as a valuable structural motif in drug design (Reissig & Zimmer, 2003; Chen *et al.*, 2012; Talele, 2016; Wu *et al.*, 2018; Bauer *et al.*, 2021). Moreover, the cyclopropyl group has also been used in supramolecular chemistry, for example in the construction of artificial receptors (Stapf *et al.*, 2020). In this paper, we describe the crystal structure of a compound bearing *N*-cyclopropylcarbamoyl groups, which belongs to the class of benzene-1,3,5-tricarboxamides. Other representatives of this class of compounds, *e.g.* those with *N*-(pyridin-2-yl)carbamoyl or *N*-(1,8-naphthyridin-2-yl)carbamoyl groups, were found to have interesting binding properties towards carbohydrates (Mazik *et al.*, 2000, 2004, 2006; Mazik & Sicking, 2001, 2004; Mazik & Cavga, 2007). It is worth noting that various supramolecular architectures based on benzene-1,3,5-tricarboxamide have been the subject of intensive research (Cantekin *et al.*, 2012). The self-aggregation processes of benzene-1,3,5-tricarboxamides have been studied particularly intensively and have led to the development of new hydrogels, hydrogen-bonded organic frameworks (HOFs) and other systems with favourable properties (Stals *et al.*, 2009; Veld *et al.*, 2011; Howe *et al.*, 2013; Kulkarni *et al.*, 2017; Li *et al.*, 2024).



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**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O3^i$	0.90 (1)	1.96 (1)	2.8471 (15)	168 (1)
$N2-H2A\cdots O2^{ii}$	0.89 (1)	1.96 (1)	2.8253 (13)	165 (2)
$N3-H3A\cdots O1^{ii}$	0.89 (1)	2.04 (1)	2.8937 (14)	159 (1)
$C2-H2\cdots O3^i$	0.95	2.58	3.3485 (17)	139
$C14-H14A\cdots O1^{iii}$	0.99	2.55	3.2839 (17)	131

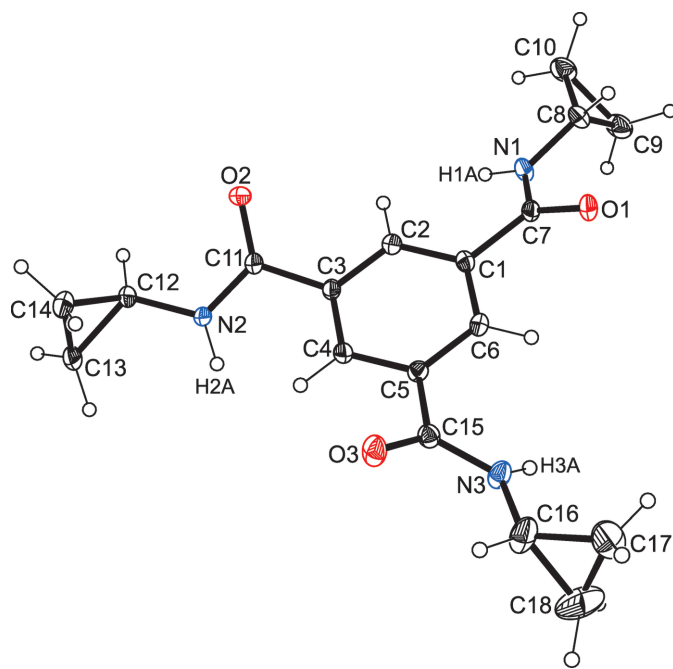
Symmetry codes: (i)  $-x, y + \frac{1}{2}, -z + \frac{1}{2}$ ; (ii)  $x + 1, y, z$ ; (iii)  $x, -y + \frac{3}{2}, z - \frac{1}{2}$ 

## 2. Structural commentary

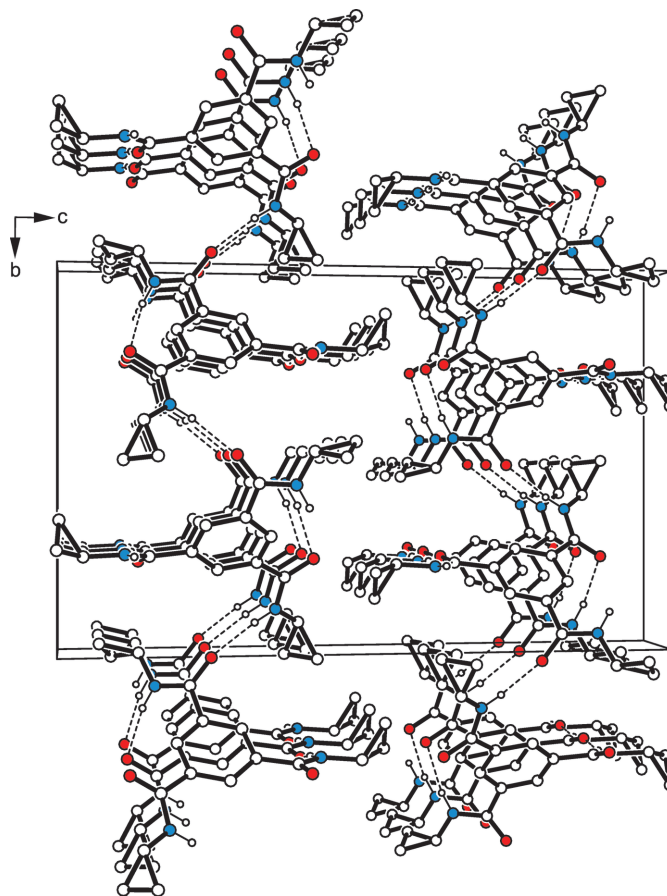
The crystal structure of the title compound,  $C_{18}H_{21}N_3O_3$ , was solved in the monoclinic space group  $P2_1/c$  with the asymmetric unit containing one molecule. One of the cyclopropyl groups is disordered over two positions (s. o. f. 0.70/0.30). The three amide units of the molecule are inclined at angles of 26.5 (1), 36.9 (1) and 37.8 (1)° with respect to the plane of the central benzene ring. This twisting, which is due to supramolecular interactions, gives the threefold-substituted benzene derivative a propeller-like conformation (Fig. 1).

## 3. Supramolecular features

In the crystal structure of the title compound, the molecules are connected by  $N-H\cdots O$  bonds [ $d(H\cdots O)$  1.96 (1)–2.04 (1) Å, 159 (1)–168 (1)°; Table 1] to form two-dimensional supramolecular networks extending parallel to the crystallographic  $ab$  plane (Figs. 2 and 3). Within these aggregates, the oxygen atom O3 participates in the formation of a  $C-H\cdots O$

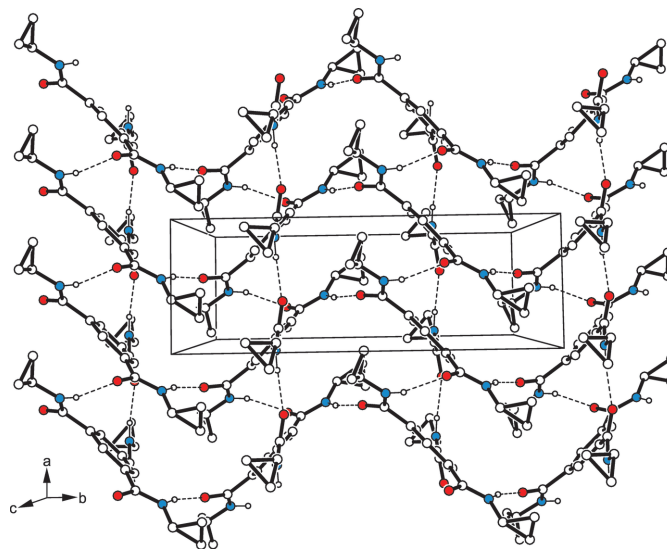
**Figure 1**

Perspective view of the title molecule including atom labelling. Anisotropic displacement ellipsoids are drawn at the 50% probability level. For the sake of clarity, only the major component of the disordered cyclopropyl ring is shown.

**Figure 2**

Packing diagram of the title compound viewed along the  $a$  axis. The  $N-H\cdots O$  hydrogen bonds are visualized as dashed lines.

bond [ $d(H\cdots O)$  2.58 Å, 139°; for other examples of  $C-H\cdots O$  bonds, see: Desiraju & Steiner, 1999; Desiraju,

**Figure 3**

Packing diagram of the title compound showing the two-dimensional supramolecular network. Dashed lines indicate  $N-H\cdots O$  hydrogen bonds.

2005; Mazik *et al.*, 1999, 2005, 2010; Ebersbach *et al.*, 2023] to the arene hydrogen H2 of an adjacent molecule. Association of the 2D networks is accomplished by C—H...O bonds involving methylene hydrogen H14A and the oxygen O1 [ $d(\text{H}\cdots\text{O})$  2.55 Å, 131°].

#### 4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.45, update June 2024; Groom *et al.*, 2016) for benzene derivatives containing at least one *N*-cycloalkylcarbamoyl group with a cyclopropyl, cyclobutyl, cyclopentyl or cyclohexyl ring gave nineteen hits. Among these are fifteen *N*-cycloalkylbenzamides, which also have other substituents on the benzene ring, such as hydroxy, methoxy or halogeno groups, making comparison difficult. For example, compounds bearing both hydroxy and methoxy groups and differing in ring size comprise *N*-cyclopropyl-3-hydroxy-4-methoxybenzamide (HOBGOY; Tong *et al.*, 2023), *N*-cyclopentyl-3-hydroxy-4-methoxybenzamide (DELLUF; Zhang *et al.*, 2022a) and *N*-cyclohexyl-3-hydroxy-4-methoxybenzamide (DELCUW; Zhang *et al.*, 2022b). The crystal structure of the compound lacking further substituents on the benzene ring is only known in the case of the cyclohexyl unit (QUZJAX; Khan *et al.*, 2010). The same applies to compounds that have two or three carboxamide units on the benzene ring; these include *N,N'*-di(cyclohexyl)benzene-1,4-dicarboxamide (DAVQUP01; Wang *et al.*, 2017) and *N,N',N''*-tris(cyclohexyl)benzene-1,3,5-tricarboxamide (CIYYAO; Li *et al.*, 2024). The latter, tripodal molecule is an analogue of the title compound, but has a markedly different crystal structure. It consists of columnar domains extending in the direction of the crystallographic *b* axis, in which the molecules are arranged in layers with a stacking of the central benzene rings. Neighbouring molecules are mainly linked by three N—H...O=C hydrogen bonds. The periphery of the domains is formed by the cyclohexyl moieties, so that they are only connected to each other *via* van der Waals interactions.

#### 5. Synthesis and crystallization

A solution of 1,3,5-benzenetricarbonyl trichloride (0.20 g, 0.75 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (10 mL) was added dropwise to a mixture of cyclopropylamine (0.18 mL, 0.15 g, 2.59 mmol) and triethylamine (0.34 mL, 0.25 g, 2.45 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (15 mL). After stirring at room temperature for 12 h, the solvent was evaporated under reduced pressure. The remaining white solid was washed several times with water, again suspended in CH<sub>2</sub>Cl<sub>2</sub>, filtered off and dried. Yield: 0.19 g (77%). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>, ppm): δ = 0.58–0.61 (*m*, 6H, CH<sub>2</sub>), 0.70–0.74 (*m*, 6H, CH<sub>2</sub>), 2.85–2.91 (*m*, 3H, CH), 8.31 (*s*, 3H, aryl), 8.65 (*d*, 3H, *J* = 4.1 Hz, NH). <sup>13</sup>C NMR (125 MHz, DMSO-*d*<sub>6</sub>, ppm): δ = 5.7 (CH<sub>2</sub>), 23.2 (CH), 128.4 (aryl), 134.8 (aryl), 166.8 (C=O). MS (ESI): *m/z* calculated for C<sub>18</sub>H<sub>22</sub>N<sub>3</sub>O<sub>3</sub>: 328.2 [*M* + H]<sup>+</sup>, found 328.1. Single crystals suitable for X-ray diffraction were obtained by crystallization of the title compound from DMSO.

**Table 2**

Experimental details.

Crystal data	
Chemical formula	C <sub>18</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub>
<i>M<sub>r</sub></i>	327.38
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.9435 (2), 14.2798 (5), 23.1247 (9)
β (°)	95.512 (2)
<i>V</i> (Å <sup>3</sup> )	1624.87 (11)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>−1</sup> )	0.09
Crystal size (mm)	0.47 × 0.11 × 0.08
Data collection	
Diffractometer	Bruker CCD area detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.958, 0.993
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	15717, 3779, 3059
<i>R</i> <sub>int</sub>	0.028
(sin θ/λ) <sub>max</sub> (Å <sup>−1</sup> )	0.652
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.040, 0.101, 1.02
No. of reflections	3779
No. of parameters	257
No. of restraints	63
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>−3</sup> )	0.36, −0.22

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015) and *ORTEP-3 for Windows* (Farrugia, 2012).

#### 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The non-hydrogen atoms were refined anisotropically. All C-bound hydrogen atoms were positioned geometrically and refined isotropically using the riding model with C—H = 0.99–1.00 Å (cycloalkyl), 0.95 Å (aryl); *U*<sub>iso</sub>(H) = 1.2–1.5*U*<sub>eq</sub>(C). The positions of the N—H hydrogens could be located in difference-Fourier maps and were refined to a target value of 0.90 Å [*U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(N)].

#### Acknowledgements

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## supporting information

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## Crystal structure of *N,N',N''*-tricyclopropylbenzene-1,3,5-tricarboxamide

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### Computing details

#### *N,N',N''*-Tricyclopropylbenzene-1,3,5-tricarboxamide

##### Crystal data

$C_{18}H_{21}N_3O_3$	$F(000) = 696$
$M_r = 327.38$	$D_x = 1.338 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 4.9435 (2) \text{ \AA}$	Cell parameters from 4588 reflections
$b = 14.2798 (5) \text{ \AA}$	$\theta = 2.9\text{--}28.5^\circ$
$c = 23.1247 (9) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$\beta = 95.512 (2)^\circ$	$T = 100 \text{ K}$
$V = 1624.87 (11) \text{ \AA}^3$	Needle, colourless
$Z = 4$	$0.47 \times 0.11 \times 0.08 \text{ mm}$

##### Data collection

Bruker CCD area detector diffractometer	3779 independent reflections
phi and $\omega$ scans	3059 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$R_{\text{int}} = 0.028$
$T_{\text{min}} = 0.958$ , $T_{\text{max}} = 0.993$	$\theta_{\text{max}} = 27.6^\circ$ , $\theta_{\text{min}} = 1.7^\circ$
15717 measured reflections	$h = -6 \rightarrow 6$
	$k = -18 \rightarrow 18$
	$l = -30 \rightarrow 30$

##### Refinement

Refinement on $F^2$	Primary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: mixed
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.101$	$w = 1/[\sigma^2(F_o^2) + (0.043P)^2 + 0.8263P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
3779 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
257 parameters	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
63 restraints	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

##### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
O1	−0.31098 (19)	0.74373 (6)	0.39186 (4)	0.0168 (2)	
O2	−0.36865 (18)	0.74689 (7)	0.12301 (4)	0.0208 (2)	
O3	0.4118 (2)	0.48708 (7)	0.26455 (4)	0.0226 (2)	
N1	−0.4171 (2)	0.86911 (8)	0.33459 (5)	0.0159 (2)	
H1A	−0.396 (3)	0.9006 (11)	0.3017 (5)	0.027 (4)*	
N2	0.0624 (2)	0.72544 (8)	0.10159 (5)	0.0156 (2)	
H2A	0.238 (2)	0.7278 (12)	0.1146 (7)	0.024 (4)*	
N3	0.5354 (2)	0.55827 (8)	0.35031 (5)	0.0198 (3)	
H3A	0.550 (3)	0.6129 (8)	0.3690 (7)	0.029 (5)*	
C1	−0.1216 (3)	0.74915 (9)	0.30131 (6)	0.0138 (3)	
C2	−0.1799 (3)	0.76665 (9)	0.24228 (6)	0.0144 (3)	
H2	−0.3183	0.8101	0.2294	0.017*	
C3	−0.0353 (3)	0.72041 (9)	0.20210 (5)	0.0138 (3)	
C4	0.1643 (3)	0.65575 (9)	0.22084 (6)	0.0145 (3)	
H4	0.2630	0.6246	0.1933	0.017*	
C5	0.2204 (3)	0.63643 (9)	0.27977 (6)	0.0140 (3)	
C6	0.0787 (3)	0.68403 (9)	0.31969 (6)	0.0142 (3)	
H6	0.1187	0.6721	0.3600	0.017*	
C7	−0.2892 (3)	0.78815 (9)	0.34647 (6)	0.0141 (3)	
C8	−0.6025 (3)	0.90605 (9)	0.37302 (6)	0.0172 (3)	
H8	−0.6957	0.8585	0.3959	0.021*	
C9	−0.5473 (3)	0.99839 (11)	0.40248 (7)	0.0257 (3)	
H9A	−0.6011	1.0060	0.4424	0.031*	
H9B	−0.3803	1.0324	0.3946	0.031*	
C10	−0.7684 (3)	0.98916 (11)	0.35391 (7)	0.0242 (3)	
H10A	−0.9587	0.9913	0.3638	0.029*	
H10B	−0.7380	1.0177	0.3161	0.029*	
C11	−0.1271 (3)	0.73253 (9)	0.13884 (6)	0.0145 (3)	
C12	−0.0096 (3)	0.73106 (10)	0.03993 (5)	0.0157 (3)	
H12	−0.1448	0.7804	0.0266	0.019*	
C13	0.2084 (3)	0.71258 (10)	0.00118 (6)	0.0198 (3)	
H13A	0.3907	0.6955	0.0196	0.024*	
H13B	0.2087	0.7505	−0.0346	0.024*	
C14	−0.0184 (3)	0.64273 (10)	0.00452 (6)	0.0194 (3)	
H14A	−0.1573	0.6381	−0.0292	0.023*	
H14B	0.0248	0.5830	0.0251	0.023*	
C15	0.4014 (3)	0.55474 (9)	0.29743 (6)	0.0157 (3)	
C16	0.7030 (9)	0.4825 (4)	0.37374 (17)	0.0243 (9)	0.700 (7)
H16	0.7408	0.4319	0.3457	0.029*	0.700 (7)
C17	0.6653 (7)	0.4516 (3)	0.43355 (16)	0.0279 (7)	0.700 (7)
H17A	0.5344	0.4867	0.4551	0.034*	0.700 (7)
H17B	0.6748	0.3836	0.4418	0.034*	0.700 (7)
C18	0.9190 (7)	0.4996 (3)	0.42163 (18)	0.0384 (8)	0.700 (7)
H18A	1.0868	0.4616	0.4225	0.046*	0.700 (7)
H18B	0.9464	0.5647	0.4357	0.046*	0.700 (7)

C16A	0.6466 (18)	0.4719 (12)	0.3775 (4)	0.0234 (15)	0.300 (7)
H16A	0.5688	0.4117	0.3613	0.028*	0.300 (7)
C17A	0.7441 (19)	0.4723 (7)	0.4401 (3)	0.0296 (14)	0.300 (7)
H17C	0.7222	0.5308	0.4621	0.036*	0.300 (7)
H17D	0.7239	0.4139	0.4623	0.036*	0.300 (7)
C18A	0.9421 (12)	0.4725 (5)	0.3963 (4)	0.0313 (13)	0.300 (7)
H18C	1.0456	0.4142	0.3911	0.038*	0.300 (7)
H18D	1.0438	0.5311	0.3910	0.038*	0.300 (7)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0226 (5)	0.0171 (5)	0.0109 (4)	0.0015 (4)	0.0031 (4)	0.0008 (4)
O2	0.0123 (5)	0.0349 (6)	0.0150 (5)	0.0026 (4)	0.0010 (4)	0.0009 (4)
O3	0.0308 (6)	0.0183 (5)	0.0184 (5)	0.0057 (4)	0.0001 (4)	−0.0049 (4)
N1	0.0197 (6)	0.0160 (5)	0.0129 (5)	0.0025 (4)	0.0056 (4)	0.0011 (4)
N2	0.0113 (5)	0.0254 (6)	0.0102 (5)	0.0005 (4)	0.0008 (4)	0.0002 (4)
N3	0.0256 (6)	0.0165 (6)	0.0161 (6)	0.0064 (5)	−0.0035 (5)	−0.0024 (5)
C1	0.0147 (6)	0.0131 (6)	0.0138 (6)	−0.0020 (5)	0.0027 (5)	−0.0017 (5)
C2	0.0137 (6)	0.0150 (6)	0.0144 (6)	0.0000 (5)	0.0006 (5)	0.0006 (5)
C3	0.0132 (6)	0.0168 (6)	0.0114 (6)	−0.0028 (5)	0.0011 (5)	−0.0005 (5)
C4	0.0132 (6)	0.0170 (6)	0.0133 (6)	−0.0008 (5)	0.0023 (5)	−0.0026 (5)
C5	0.0139 (6)	0.0138 (6)	0.0139 (6)	−0.0008 (5)	−0.0001 (5)	−0.0006 (5)
C6	0.0165 (6)	0.0152 (6)	0.0107 (6)	−0.0017 (5)	0.0001 (5)	−0.0002 (5)
C7	0.0151 (6)	0.0152 (6)	0.0119 (6)	−0.0013 (5)	0.0004 (5)	−0.0021 (5)
C8	0.0181 (6)	0.0176 (7)	0.0168 (7)	0.0019 (5)	0.0070 (5)	0.0003 (5)
C9	0.0220 (7)	0.0275 (8)	0.0287 (8)	0.0001 (6)	0.0075 (6)	−0.0113 (6)
C10	0.0227 (7)	0.0253 (7)	0.0255 (8)	0.0083 (6)	0.0068 (6)	0.0026 (6)
C11	0.0148 (6)	0.0166 (6)	0.0120 (6)	−0.0005 (5)	0.0013 (5)	−0.0002 (5)
C12	0.0157 (6)	0.0212 (7)	0.0103 (6)	0.0015 (5)	0.0013 (5)	0.0009 (5)
C13	0.0192 (7)	0.0273 (7)	0.0132 (6)	−0.0021 (5)	0.0039 (5)	−0.0022 (5)
C14	0.0227 (7)	0.0209 (7)	0.0143 (6)	−0.0018 (5)	−0.0004 (5)	−0.0005 (5)
C15	0.0176 (6)	0.0148 (6)	0.0150 (6)	0.0009 (5)	0.0031 (5)	−0.0003 (5)
C16	0.0310 (18)	0.0239 (19)	0.0174 (11)	0.0150 (16)	−0.0016 (12)	0.0002 (10)
C17	0.0242 (15)	0.0277 (15)	0.0317 (14)	0.0028 (11)	0.0015 (11)	0.0114 (11)
C18	0.0327 (14)	0.0422 (17)	0.0365 (17)	−0.0049 (12)	−0.0162 (13)	0.0200 (13)
C16A	0.022 (3)	0.019 (3)	0.028 (3)	0.003 (2)	−0.003 (2)	0.002 (2)
C17A	0.032 (3)	0.029 (3)	0.027 (2)	0.010 (2)	−0.002 (2)	0.007 (2)
C18A	0.022 (2)	0.027 (2)	0.044 (3)	0.0003 (19)	0.001 (2)	0.015 (2)

*Geometric parameters (Å, °)*

O1—C7	1.2400 (16)	C9—H9A	0.9900
O2—C11	1.2321 (16)	C9—H9B	0.9900
O3—C15	1.2337 (16)	C10—H10A	0.9900
N1—C7	1.3334 (17)	C10—H10B	0.9900
N1—C8	1.4369 (16)	C12—C13	1.4896 (18)
N1—H1A	0.897 (9)	C12—C14	1.5023 (19)

N2—C11	1.3361 (16)	C12—H12	1.0000
N2—C12	1.4381 (16)	C13—C14	1.5080 (19)
N2—H2A	0.893 (9)	C13—H13A	0.9900
N3—C15	1.3346 (17)	C13—H13B	0.9900
N3—C16	1.437 (6)	C14—H14A	0.9900
N3—C16A	1.467 (15)	C14—H14B	0.9900
N3—H3A	0.891 (9)	C16—C17	1.481 (5)
C1—C2	1.3903 (18)	C16—C18	1.483 (4)
C1—C6	1.3948 (18)	C16—H16	1.0000
C1—C7	1.5010 (17)	C17—C18	1.479 (4)
C2—C3	1.3921 (18)	C17—H17A	0.9900
C2—H2	0.9500	C17—H17B	0.9900
C3—C4	1.3899 (18)	C18—H18A	0.9900
C3—C11	1.4996 (18)	C18—H18B	0.9900
C4—C5	1.3921 (18)	C16A—C17A	1.481 (9)
C4—H4	0.9500	C16A—C18A	1.483 (8)
C5—C6	1.3889 (18)	C16A—H16A	1.0000
C5—C15	1.5026 (18)	C17A—C18A	1.474 (8)
C6—H6	0.9500	C17A—H17C	0.9900
C8—C10	1.4854 (19)	C17A—H17D	0.9900
C8—C9	1.497 (2)	C18A—H18C	0.9900
C8—H8	1.0000	C18A—H18D	0.9900
C9—C10	1.496 (2)		
C7—N1—C8	120.59 (11)	C13—C12—C14	60.53 (9)
C7—N1—H1A	121.2 (11)	N2—C12—H12	116.1
C8—N1—H1A	118.2 (11)	C13—C12—H12	116.1
C11—N2—C12	120.85 (11)	C14—C12—H12	116.1
C11—N2—H2A	120.0 (11)	C12—C13—C14	60.15 (9)
C12—N2—H2A	118.2 (11)	C12—C13—H13A	117.8
C15—N3—C16	122.3 (2)	C14—C13—H13A	117.8
C15—N3—C16A	119.6 (5)	C12—C13—H13B	117.8
C15—N3—H3A	119.2 (12)	C14—C13—H13B	117.8
C16—N3—H3A	117.3 (12)	H13A—C13—H13B	114.9
C16A—N3—H3A	121.2 (13)	C12—C14—C13	59.32 (9)
C2—C1—C6	119.55 (12)	C12—C14—H14A	117.8
C2—C1—C7	122.69 (12)	C13—C14—H14A	117.8
C6—C1—C7	117.28 (11)	C12—C14—H14B	117.8
C1—C2—C3	119.91 (12)	C13—C14—H14B	117.8
C1—C2—H2	120.0	H14A—C14—H14B	115.0
C3—C2—H2	120.0	O3—C15—N3	123.22 (13)
C4—C3—C2	120.12 (12)	O3—C15—C5	119.98 (12)
C4—C3—C11	121.33 (11)	N3—C15—C5	116.73 (11)
C2—C3—C11	118.02 (12)	N3—C16—C17	117.2 (4)
C3—C4—C5	120.37 (12)	N3—C16—C18	120.4 (4)
C3—C4—H4	119.8	C17—C16—C18	59.9 (2)
C5—C4—H4	119.8	N3—C16—H16	115.9
C6—C5—C4	119.21 (12)	C17—C16—H16	115.9



C6—C5—C15	121.63 (12)	C18—C16—H16	115.9
C4—C5—C15	118.51 (11)	C18—C17—C16	60.1 (2)
C5—C6—C1	120.82 (12)	C18—C17—H17A	117.8
C5—C6—H6	119.6	C16—C17—H17A	117.8
C1—C6—H6	119.6	C18—C17—H17B	117.8
O1—C7—N1	122.67 (12)	C16—C17—H17B	117.8
O1—C7—C1	119.86 (12)	H17A—C17—H17B	114.9
N1—C7—C1	117.43 (11)	C17—C18—C16	60.0 (2)
N1—C8—C10	118.44 (12)	C17—C18—H18A	117.8
N1—C8—C9	120.37 (12)	C16—C18—H18A	117.8
C10—C8—C9	60.20 (10)	C17—C18—H18B	117.8
N1—C8—H8	115.5	C16—C18—H18B	117.8
C10—C8—H8	115.5	H18A—C18—H18B	114.9
C9—C8—H8	115.5	N3—C16A—C17A	119.3 (12)
C10—C9—C8	59.51 (10)	N3—C16A—C18A	116.1 (9)
C10—C9—H9A	117.8	C17A—C16A—C18A	59.6 (4)
C8—C9—H9A	117.8	N3—C16A—H16A	116.6
C10—C9—H9B	117.8	C17A—C16A—H16A	116.6
C8—C9—H9B	117.8	C18A—C16A—H16A	116.6
H9A—C9—H9B	115.0	C18A—C17A—C16A	60.3 (4)
C8—C10—C9	60.29 (10)	C18A—C17A—H17C	117.7
C8—C10—H10A	117.7	C16A—C17A—H17C	117.7
C9—C10—H10A	117.7	C18A—C17A—H17D	117.7
C8—C10—H10B	117.7	C16A—C17A—H17D	117.7
C9—C10—H10B	117.7	H17C—C17A—H17D	114.9
H10A—C10—H10B	114.9	C17A—C18A—C16A	60.1 (4)
O2—C11—N2	122.73 (12)	C17A—C18A—H18C	117.8
O2—C11—C3	120.18 (11)	C16A—C18A—H18C	117.8
N2—C11—C3	117.07 (11)	C17A—C18A—H18D	117.8
N2—C12—C13	117.52 (11)	C16A—C18A—H18D	117.8
N2—C12—C14	119.02 (11)	H18C—C18A—H18D	114.9
C6—C1—C2—C3	-1.09 (19)	C4—C3—C11—O2	141.84 (13)
C7—C1—C2—C3	-173.04 (12)	C2—C3—C11—O2	-29.81 (18)
C1—C2—C3—C4	0.99 (19)	C4—C3—C11—N2	-37.08 (18)
C1—C2—C3—C11	172.74 (11)	C2—C3—C11—N2	151.28 (12)
C2—C3—C4—C5	0.26 (19)	C11—N2—C12—C13	-173.74 (12)
C11—C3—C4—C5	-171.21 (12)	C11—N2—C12—C14	-103.94 (15)
C3—C4—C5—C6	-1.40 (19)	N2—C12—C13—C14	109.50 (13)
C3—C4—C5—C15	169.51 (12)	N2—C12—C14—C13	-107.07 (13)
C4—C5—C6—C1	1.30 (19)	C16—N3—C15—O3	-0.5 (3)
C15—C5—C6—C1	-169.32 (12)	C16A—N3—C15—O3	-15.6 (5)
C2—C1—C6—C5	-0.06 (19)	C16—N3—C15—C5	176.5 (2)
C7—C1—C6—C5	172.32 (12)	C16A—N3—C15—C5	161.4 (5)
C8—N1—C7—O1	-4.0 (2)	C6—C5—C15—O3	142.42 (13)
C8—N1—C7—C1	173.74 (11)	C4—C5—C15—O3	-28.26 (18)
C2—C1—C7—O1	149.28 (13)	C6—C5—C15—N3	-34.62 (18)
C6—C1—C7—O1	-22.83 (18)	C4—C5—C15—N3	154.70 (12)

C2—C1—C7—N1	-28.51 (18)	C15—N3—C16—C17	-132.1 (4)
C6—C1—C7—N1	159.38 (12)	C15—N3—C16—C18	158.6 (3)
C7—N1—C8—C10	-171.59 (13)	N3—C16—C17—C18	-111.1 (4)
C7—N1—C8—C9	118.15 (15)	N3—C16—C18—C17	105.8 (4)
N1—C8—C9—C10	107.48 (14)	C15—N3—C16A—C17A	-167.5 (7)
N1—C8—C10—C9	-110.63 (14)	C15—N3—C16A—C18A	124.3 (8)
C12—N2—C11—O2	-2.3 (2)	N3—C16A—C17A—C18A	-104.8 (9)
C12—N2—C11—C3	176.63 (12)	N3—C16A—C18A—C17A	110.2 (12)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1A $\cdots$ O3 <sup>i</sup>	0.90 (1)	1.96 (1)	2.8471 (15)	168 (1)
N2—H2A $\cdots$ O2 <sup>ii</sup>	0.89 (1)	1.96 (1)	2.8253 (13)	165 (2)
N3—H3A $\cdots$ O1 <sup>ii</sup>	0.89 (1)	2.04 (1)	2.8937 (14)	159 (1)
C2—H2 $\cdots$ O3 <sup>i</sup>	0.95	2.58	3.3485 (17)	139
C14—H14A $\cdots$ O1 <sup>iii</sup>	0.99	2.55	3.2839 (17)	131

Symmetry codes: (i)  $-x, y+1/2, -z+1/2$ ; (ii)  $x+1, y, z$ ; (iii)  $x, -y+3/2, z-1/2$ .