IUCrData

ISSN 2414-3146

3,3′-[(Cyclohexane-1,4-diyl)bis(azanediyl)]bis-(cyclohex-2-en-1-one)

Antar A. Abdelhamida,[a] Shaaban K. Mohamed[a] and Jim Simpson[b]*

[a]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, and [b]Department of Chemistry, University of Otago, PO Box 56, Dunedin, New Zealand. *Correspondence e-mail: jsimpson@alkali.otago.ac.nz

Received 29 October 2015
Accepted 16 November 2015

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

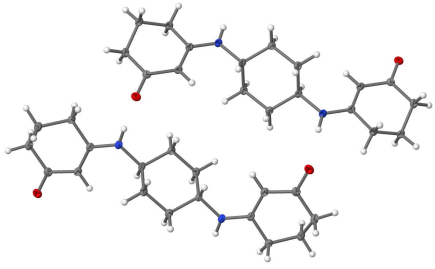
Keywords: crystal structure; cyclohexane-1,4-diamine; cyclohexane-1,3-dione; acetamide; hydrogen bonding; inversion dimers.

CCDC reference: 1440892

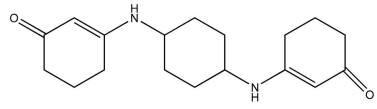
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{18}H_{26}N_2O_2$, crystallizes with two half-molecules in the asymmetric unit, both lying about inversion centres situated at the centers of the cyclohexane rings. In the crystal, the two molecules are linked by a pair of N—H···O hydrogen bonds, forming an inversion dimer with an $R_2^2(18)$ ring motif; the dimers are linked by a second pair of N—H···O hydrogen bonds, enclosing an $R_2^2(18)$ ring motif, forming chains along [1$\bar{1}$0] which are linked by bifurcated C—H···(O,O) hydrogen bonds, forming slabs parallel to the *ab* plane.

3D view



Chemical scheme



Structure description

The title compound, $C_{18}H_{26}N_2O_2$, was prepared by a direct condensation reaction between cyclohexane-1,4-diamine and cyclohexane-1,3-dione to afford the corresponding symmetrical diamine. It crystallizes with two half-molecules in the asymmetric unit, both lying about inversion centres situated at the centers of the cyclohexane rings. In the two molecules (1 and 2; Fig. 1) the central cyclohexane rings adopt chair conformations and are linked by NH bridges to two cyclohexenone rings. The latter each display envelope conformations with the central methylene C atoms of the CH_2–CH_2–CH_2 segment as the flaps. The adjacent C═C and C—N bond distances of 1.3771 (16) and 1.3394 (15) Å, respectively, for molecule 1, and 1.3803 (15) and 1.3375 (14) Å, respectively, for molecule 2, indicate a considerable degree of delocalization across the C—N bonds. In the crystal, the two molecules are linked by a pair of N—H···O hydrogen bonds, forming an inversion dimer with an $R_2^2(18)$ ring motif (Table 1 and Fig. 2). These dimers are linked by a second pair of N—H···O hydrogen bonds, enclosing an $R_2^2(18)$ ring motif, forming chains along [1$\bar{1}$0]; Table 1 and Fig. 2. The chains are linked by bifurcated C—H···(O,O) hydrogen bonds, forming slabs parallel to the *ab* plane (Table 1 and Fig. 3).

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11*N*···O21′	0.896 (16)	1.944 (16)	2.8369 (13)	174.8 (14)
N21—H21*N*···O11′^{i}	0.884 (15)	2.012 (15)	2.8930 (13)	174.1 (13)
C21—H21···O21′^{ii}	1.00	2.59	3.4511 (13)	144
C22—H22*B*···O21′^{iii}	0.99	2.50	3.3675 (14)	147

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

No structures of derivatives of cyclohexane-1,4-diamine with either cyclohexene or cyclohexane substituents on the N atoms appear in the literature. The closest relatives of the title compound in the Cambridge Structural Database (Groom & Allen, 2014) are found as Ru complexes of ligands that have either a phenyl ring on one N atom of the central cyclohexane-1,4-diamine unit and a benzyl substituent on the other (Samec *et al.*, 2006) or alternatively benzyl substituents on both N atoms (Casey *et al.*, 2007).

Synthesis and crystallization

A mixture of 114 mg (0.1 mmol) of cyclohexane-1,4-diamine and 112 mg (0.1 mmol) of cyclohexane-1,3-dione was refluxed at 352 K in 30 ml ethanol. The reaction was monitored by TLC, was complete after 5 h and left to cool to room temperature. The excess solvent was evaporated under vacuum and the resulting solid filtered off, dried and recrystallized from acetic acid (m.p. 593 K). Crystals suitable for X-ray data collection were grown by slow evaporation of a solution of acetic acid over four days at ambient temperature.

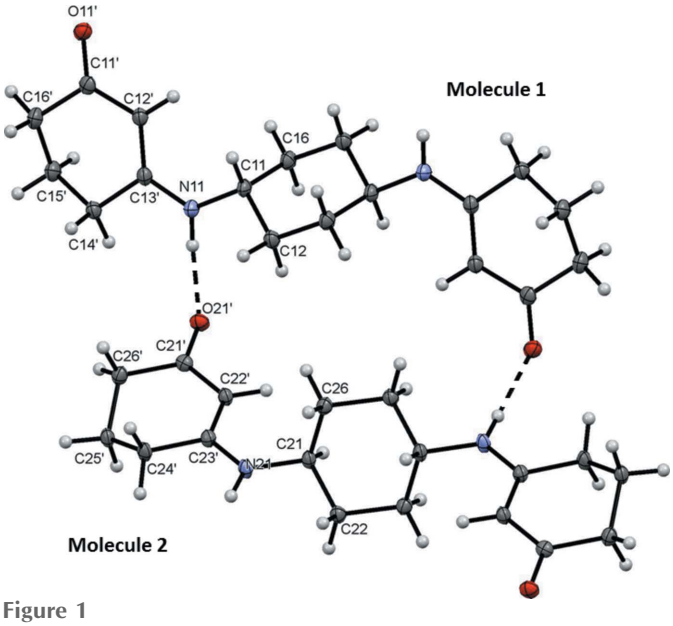


Figure 1
The molecular structure of the two independent molecules (1 and 2) of the title compound. Displacement ellipsoids are drawn at the 50% probability level. The N—H···O hydrogen bonds are shown as dashed lines (see Table 1), and unlabelled atoms are related to labelled atoms by symmetry operations $-x+1, -y+1, -z+1$ for molecule 1 and $-x+2, -y, -z+1$ for molecule 2.

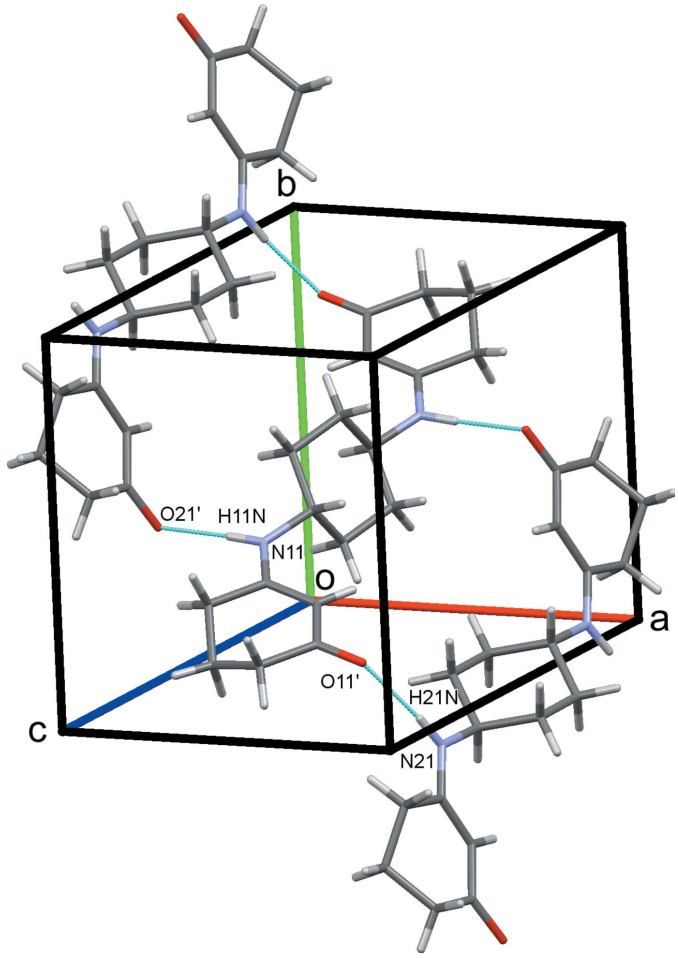


Figure 2
A view along the normal to the *ab* plane of the hydrogen-bonded chain of molecules 1 and 2 of the title compound (dashed lines; see Table 1).

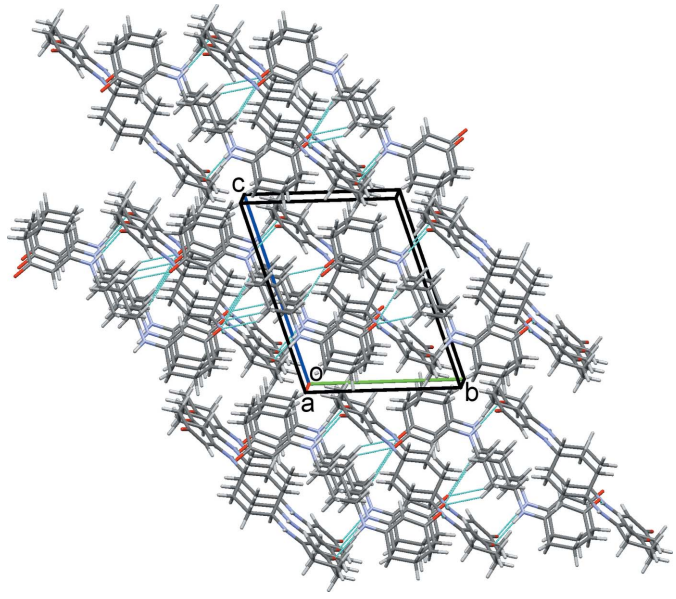


Figure 3
A view along the *a* axis of the crystal packing of the title compound with hydrogen bonds shown as dashed lines (see Table 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{26}N_2O_2$
M_r	302.41
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	8.1839 (2), 9.1461 (3), 11.7669 (4)
α, β, γ (°)	106.557 (3), 97.687 (2), 96.630 (2)
V (Å^3)	825.65 (5)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.63
Crystal size (mm)	0.54 × 0.35 × 0.07
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
Absorption correction	Multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min}, T_{max}	0.845, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12078, 3272, 3002
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.103, 1.10
No. of reflections	3272
No. of parameters	219
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, −0.30

Computer programs: *CrysAlis PRO*, Agilent (2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*) and *TITAN2000* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009), *publCIF* (Westrip 2010), *WinGX* (Farrugia 2012).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

We thank the University of Otago for the purchase of the diffractometer and the Chemistry Department, University of Otago, for support of the work of JS. SKM thanks Dr Alaa F. Mohamed, National Organization for Drug Control and Research (NODCAR), Egypt, for providing the necessary chemicals.

References

Agilent (2013). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.

Casey, C. P., Clark, T. B. & Guzei, I. A. (2007). *J. Am. Chem. Soc.* **129**, 11821–11827.

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.

Groom, C. R. & Allen, F. H. (2014). *Angew. Chem. Int. Ed.* **53**, 662–671.

Hunter, K. A. & Simpson, J. (1999). *TITAN2000*. University of Otago, New Zealand.

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.

Samec, J. S. M., Éll, A. H., Åberg, J. B., Privalov, T., Eriksson, L. & Bäckvall, J.-E. (2006). *J. Am. Chem. Soc.* **128**, 14293–14305.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2016). **1**, x152175 [https://doi.org/10.1107/S2414314615021756]

3,3′-[(Cyclohexane-1,4-diyl)bis(azanediyl)]bis(cyclohex-2-en-1-one)

Antar A. Abdelhamida, Shaaban K. Mohamed and Jim Simpson

3,3′-[(Cyclohexane-1,4-diyl)bis(azanediyl)]bis(cyclohex-2-en-1-one)

Crystal data

$C_{18}H_{26}N_2O_2$
M_r = 302.41
Triclinic, $P\overline{1}$
a = 8.1839 (2) Å
b = 9.1461 (3) Å
c = 11.7669 (4) Å
α = 106.557 (3)°
β = 97.687 (2)°
γ = 96.630 (2)°
V = 825.65 (5) Å^3
Z = 2
$F(000)$ = 328
D_x = 1.216 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 9205 reflections
θ = 4.0–74.1°
μ = 0.63 mm^{-1}
T = 100 K
Plate, orange
0.54 × 0.35 × 0.07 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
Mirror monochromator
Detector resolution: 5.1725 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Agilent, 2013)
T_{min} = 0.845, T_{max} = 1.000
12078 measured reflections
3272 independent reflections
3002 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 74.1°, θ_{min} = 4.0°
h = −9→10
k = −11→11
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.10
3272 reflections
219 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.2392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O11′	0.17860 (10)	0.83044 (9)	0.13490 (7)	0.0202 (2)
C11′	0.32063 (14)	0.79299 (12)	0.14231 (9)	0.0170 (2)
C12′	0.38277 (14)	0.72110 (13)	0.22838 (10)	0.0177 (2)
H12′	0.3140	0.7018	0.2832	0.021*
C13′	0.53902 (14)	0.67872 (12)	0.23469 (9)	0.0162 (2)
N11	0.59935 (12)	0.60257 (11)	0.30855 (9)	0.0184 (2)
H11N	0.708 (2)	0.5950 (16)	0.3150 (13)	0.022*
C11	0.50682 (13)	0.54283 (13)	0.38859 (10)	0.0165 (2)
H11	0.3873	0.5081	0.3483	0.020*
C12	0.57883 (15)	0.40283 (13)	0.40741 (10)	0.0187 (2)
H12A	0.6989	0.4342	0.4432	0.022*
H12B	0.5690	0.3230	0.3286	0.022*
C16	0.51340 (15)	0.66504 (13)	0.50964 (10)	0.0181 (2)
H161	0.6304 (17)	0.7022 (15)	0.5469 (12)	0.016 (3)*
H162	0.4644 (18)	0.7539 (16)	0.4973 (13)	0.022 (3)*
C14′	0.65503 (14)	0.71158 (13)	0.15190 (10)	0.0180 (2)
H14A	0.6440	0.6187	0.0813	0.022*
H14B	0.7719	0.7339	0.1950	0.022*
C15′	0.61656 (15)	0.84812 (14)	0.10889 (10)	0.0208 (3)
H15A	0.6848	0.8584	0.0474	0.025*
H15B	0.6452	0.9446	0.1774	0.025*
C16′	0.43164 (15)	0.82319 (14)	0.05536 (11)	0.0224 (3)
H16C	0.4059	0.9159	0.0335	0.027*
H16D	0.4072	0.7342	−0.0192	0.027*
O21′	0.94724 (10)	0.59292 (9)	0.34302 (7)	0.01825 (19)
C21′	0.98783 (13)	0.47129 (12)	0.28124 (9)	0.0147 (2)
C22′	1.01924 (13)	0.34896 (12)	0.32908 (9)	0.0154 (2)
H22′	1.0180	0.3630	0.4121	0.018*
C23′	1.05146 (13)	0.21036 (12)	0.25822 (9)	0.0148 (2)
N21	1.07308 (12)	0.08956 (11)	0.29800 (8)	0.0164 (2)
H21N	1.0982 (17)	0.0065 (17)	0.2477 (13)	0.020*
C21	1.05449 (14)	0.08363 (12)	0.41861 (9)	0.0149 (2)
H21	1.1054	0.1860	0.4782	0.018*
C22	1.14853 (14)	−0.03970 (12)	0.44659 (9)	0.0162 (2)
H22A	1.2683	−0.0137	0.4433	0.019*
H22B	1.1038	−0.1409	0.3854	0.019*
C26	0.86983 (14)	0.05044 (13)	0.42843 (10)	0.0165 (2)
H261	0.8108 (17)	0.1327 (16)	0.4127 (13)	0.020*
H262	0.8183 (17)	−0.0501 (16)	0.3656 (13)	0.020*
C24′	1.06061 (15)	0.18458 (12)	0.12708 (9)	0.0173 (2)
H24A	0.9503	0.1330	0.0778	0.021*
H24B	1.1429	0.1152	0.1038	0.021*
C25′	1.11107 (14)	0.33592 (13)	0.10069 (9)	0.0175 (2)
H25A	1.2290	0.3788	0.1382	0.021*
H25B	1.1011	0.3163	0.0127	0.021*

C26′	0.99899 (14)	0.45218 (12)	0.15038 (10)	0.0174 (2)
H26A	1.0428	0.5537	0.1425	0.021*
H26B	0.8854	0.4178	0.1015	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11′	0.0246 (4)	0.0202 (4)	0.0159 (4)	0.0097 (3)	0.0022 (3)	0.0037 (3)
C11′	0.0223 (5)	0.0138 (5)	0.0131 (5)	0.0037 (4)	0.0020 (4)	0.0016 (4)
C12′	0.0214 (5)	0.0193 (6)	0.0148 (5)	0.0051 (4)	0.0056 (4)	0.0073 (4)
C13′	0.0218 (5)	0.0148 (5)	0.0130 (5)	0.0031 (4)	0.0046 (4)	0.0050 (4)
N11	0.0185 (5)	0.0239 (5)	0.0185 (5)	0.0067 (4)	0.0064 (4)	0.0126 (4)
C11	0.0173 (5)	0.0198 (6)	0.0160 (5)	0.0034 (4)	0.0043 (4)	0.0103 (4)
C12	0.0237 (6)	0.0194 (6)	0.0167 (5)	0.0068 (4)	0.0075 (4)	0.0085 (4)
C16	0.0223 (6)	0.0173 (5)	0.0180 (5)	0.0045 (4)	0.0051 (4)	0.0091 (4)
C14′	0.0218 (5)	0.0198 (6)	0.0159 (5)	0.0059 (4)	0.0074 (4)	0.0081 (4)
C15′	0.0239 (6)	0.0225 (6)	0.0208 (5)	0.0049 (5)	0.0069 (4)	0.0123 (5)
C16′	0.0266 (6)	0.0264 (6)	0.0189 (5)	0.0062 (5)	0.0046 (5)	0.0133 (5)
O21′	0.0216 (4)	0.0141 (4)	0.0189 (4)	0.0054 (3)	0.0055 (3)	0.0029 (3)
C21′	0.0141 (5)	0.0138 (5)	0.0149 (5)	0.0012 (4)	0.0023 (4)	0.0028 (4)
C22′	0.0197 (5)	0.0156 (5)	0.0115 (5)	0.0036 (4)	0.0047 (4)	0.0039 (4)
C23′	0.0173 (5)	0.0145 (5)	0.0125 (5)	0.0023 (4)	0.0034 (4)	0.0038 (4)
N21	0.0267 (5)	0.0130 (5)	0.0108 (4)	0.0062 (4)	0.0066 (4)	0.0031 (4)
C21	0.0211 (5)	0.0133 (5)	0.0109 (5)	0.0034 (4)	0.0043 (4)	0.0038 (4)
C22	0.0197 (5)	0.0160 (5)	0.0150 (5)	0.0046 (4)	0.0056 (4)	0.0062 (4)
C26	0.0192 (5)	0.0169 (5)	0.0147 (5)	0.0041 (4)	0.0027 (4)	0.0066 (4)
C24′	0.0263 (6)	0.0153 (5)	0.0108 (5)	0.0063 (4)	0.0054 (4)	0.0028 (4)
C25′	0.0248 (6)	0.0181 (5)	0.0119 (5)	0.0056 (4)	0.0062 (4)	0.0057 (4)
C26′	0.0229 (6)	0.0157 (5)	0.0144 (5)	0.0047 (4)	0.0024 (4)	0.0057 (4)

Geometric parameters (Å, º)

O11′—C11′	1.2481 (14)	O21′—C21′	1.2512 (13)
C11′—C12′	1.4267 (15)	C21′—C22′	1.4217 (15)
C11′—C16′	1.5167 (15)	C21′—C26′	1.5159 (14)
C12′—C13′	1.3771 (16)	C22′—C23′	1.3803 (15)
C12′—H12′	0.9500	C22′—H22′	0.9500
C13′—N11	1.3394 (15)	C23′—N21	1.3375 (14)
C13′—C14′	1.5131 (15)	C23′—C24′	1.5067 (14)
N11—C11	1.4654 (13)	N21—C21	1.4629 (13)
N11—H11N	0.896 (16)	N21—H21N	0.884 (15)
C11—C12	1.5287 (15)	C21—C22	1.5223 (15)
C11—C16	1.5295 (16)	C21—C26	1.5330 (15)
C11—H11	1.0000	C21—H21	1.0000
C12—C16^{i}	1.5303 (14)	C22—C26^{ii}	1.5274 (14)
C12—H12A	0.9900	C22—H22A	0.9900
C12—H12B	0.9900	C22—H22B	0.9900
C16—C12^{i}	1.5303 (14)	C26—C22^{ii}	1.5274 (14)

C16—H161	0.976 (14)	C26—H261	0.987 (15)
C16—H162	0.984 (15)	C26—H262	1.005 (14)
C14′—C15′	1.5241 (15)	C24′—C25′	1.5264 (15)
C14′—H14A	0.9900	C24′—H24A	0.9900
C14′—H14B	0.9900	C24′—H24B	0.9900
C15′—C16′	1.5240 (17)	C25′—C26′	1.5259 (15)
C15′—H15A	0.9900	C25′—H25A	0.9900
C15′—H15B	0.9900	C25′—H25B	0.9900
C16′—H16C	0.9900	C26′—H26A	0.9900
C16′—H16D	0.9900	C26′—H26B	0.9900
O11′—C11′—C12′	122.81 (10)	O21′—C21′—C22′	122.03 (10)
O11′—C11′—C16′	118.83 (10)	O21′—C21′—C26′	118.86 (9)
C12′—C11′—C16′	118.36 (10)	C22′—C21′—C26′	119.09 (9)
C13′—C12′—C11′	122.23 (10)	C23′—C22′—C21′	121.82 (10)
C13′—C12′—H12′	118.9	C23′—C22′—H22′	119.1
C11′—C12′—H12′	118.9	C21′—C22′—H22′	119.1
N11—C13′—C12′	124.62 (10)	N21—C23′—C22′	123.77 (10)
N11—C13′—C14′	114.55 (10)	N21—C23′—C24′	115.16 (9)
C12′—C13′—C14′	120.79 (10)	C22′—C23′—C24′	121.05 (10)
C13′—N11—C11	125.64 (10)	C23′—N21—C21	124.53 (9)
C13′—N11—H11N	117.4 (9)	C23′—N21—H21N	118.1 (9)
C11—N11—H11N	116.7 (9)	C21—N21—H21N	117.4 (9)
N11—C11—C12	108.57 (9)	N21—C21—C22	108.82 (9)
N11—C11—C16	112.30 (9)	N21—C21—C26	111.15 (9)
C12—C11—C16	110.44 (9)	C22—C21—C26	110.89 (9)
N11—C11—H11	108.5	N21—C21—H21	108.6
C12—C11—H11	108.5	C22—C21—H21	108.6
C16—C11—H11	108.5	C26—C21—H21	108.6
C11—C12—C16^{i}	110.98 (9)	C21—C22—C26^{ii}	110.27 (9)
C11—C12—H12A	109.4	C21—C22—H22A	109.6
C16^{i}—C12—H12A	109.4	C26^{ii}—C22—H22A	109.6
C11—C12—H12B	109.4	C21—C22—H22B	109.6
C16^{i}—C12—H12B	109.4	C26^{ii}—C22—H22B	109.6
H12A—C12—H12B	108.0	H22A—C22—H22B	108.1
C11—C16—C12^{i}	110.90 (9)	C22^{ii}—C26—C21	110.87 (9)
C11—C16—H161	108.2 (8)	C22^{ii}—C26—H261	109.2 (8)
C12^{i}—C16—H161	109.8 (8)	C21—C26—H261	110.3 (8)
C11—C16—H162	110.2 (8)	C22^{ii}—C26—H262	109.8 (8)
C12^{i}—C16—H162	110.0 (8)	C21—C26—H262	108.1 (8)
H161—C16—H162	107.6 (11)	H261—C26—H262	108.5 (11)
C13′—C14′—C15′	111.81 (9)	C23′—C24′—C25′	111.93 (9)
C13′—C14′—H14A	109.3	C23′—C24′—H24A	109.2
C15′—C14′—H14A	109.3	C25′—C24′—H24A	109.2
C13′—C14′—H14B	109.3	C23′—C24′—H24B	109.2
C15′—C14′—H14B	109.3	C25′—C24′—H24B	109.2
H14A—C14′—H14B	107.9	H24A—C24′—H24B	107.9
C14′—C15′—C16′	109.70 (9)	C26′—C25′—C24′	110.10 (9)

C14′—C15′—H15A	109.7	C26′—C25′—H25A	109.6
C16′—C15′—H15A	109.7	C24′—C25′—H25A	109.6
C14′—C15′—H15B	109.7	C26′—C25′—H25B	109.6
C16′—C15′—H15B	109.7	C24′—C25′—H25B	109.6
H15A—C15′—H15B	108.2	H25A—C25′—H25B	108.2
C11′—C16′—C15′	112.08 (9)	C21′—C26′—C25′	112.89 (9)
C11′—C16′—H16C	109.2	C21′—C26′—H26A	109.0
C15′—C16′—H16C	109.2	C25′—C26′—H26A	109.0
C11′—C16′—H16D	109.2	C21′—C26′—H26B	109.0
C15′—C16′—H16D	109.2	C25′—C26′—H26B	109.0
H16C—C16′—H16D	107.9	H26A—C26′—H26B	107.8
O11′—C11′—C12′—C13′	179.23 (10)	O21′—C21′—C22′—C23′	174.96 (10)
C16′—C11′—C12′—C13′	−0.02 (16)	C26′—C21′—C22′—C23′	−3.27 (16)
C11′—C12′—C13′—N11	−175.70 (10)	C21′—C22′—C23′—N21	−176.41 (10)
C11′—C12′—C13′—C14′	1.92 (17)	C21′—C22′—C23′—C24′	2.13 (16)
C12′—C13′—N11—C11	4.30 (18)	C22′—C23′—N21—C21	4.36 (17)
C14′—C13′—N11—C11	−173.45 (10)	C24′—C23′—N21—C21	−174.25 (9)
C13′—N11—C11—C12	152.07 (11)	C23′—N21—C21—C22	−159.15 (10)
C13′—N11—C11—C16	−85.51 (13)	C23′—N21—C21—C26	78.46 (13)
N11—C11—C12—C16^{i}	−179.88 (9)	N21—C21—C22—C26^{ii}	−179.35 (8)
C16—C11—C12—C16^{i}	56.59 (13)	C26—C21—C22—C26^{ii}	−56.80 (12)
N11—C11—C16—C12^{i}	−177.89 (9)	N21—C21—C26—C22^{ii}	178.33 (9)
C12—C11—C16—C12^{i}	−56.54 (13)	C22—C21—C26—C22^{ii}	57.15 (12)
N11—C13′—C14′—C15′	−156.94 (10)	N21—C23′—C24′—C25′	−155.02 (10)
C12′—C13′—C14′—C15′	25.22 (14)	C22′—C23′—C24′—C25′	26.32 (14)
C13′—C14′—C15′—C16′	−52.41 (13)	C23′—C24′—C25′—C26′	−51.78 (12)
O11′—C11′—C16′—C15′	151.78 (10)	O21′—C21′—C26′—C25′	157.43 (10)
C12′—C11′—C16′—C15′	−28.93 (14)	C22′—C21′—C26′—C25′	−24.28 (14)
C14′—C15′—C16′—C11′	54.51 (13)	C24′—C25′—C26′—C21′	51.07 (12)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N11—H11*N*···O21′	0.896 (16)	1.944 (16)	2.8369 (13)	174.8 (14)
N21—H21*N*···O11′^{iii}	0.884 (15)	2.012 (15)	2.8930 (13)	174.1 (13)
C21—H21···O21′^{iv}	1.00	2.59	3.4511 (13)	144
C22—H22*B*···O21′^{v}	0.99	2.50	3.3675 (14)	147

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