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A 1:1 molecular complex of dicyclohexylamine and cyclohexanone oxime

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.094
Data-to-parameter ratio = 6.5

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

The molecules of the title complex, $C_{12}H_{23}N{\cdot}C_6H_{11}N$, are linked together in chains by O—H···N and N—H···O hydrogen bonds.

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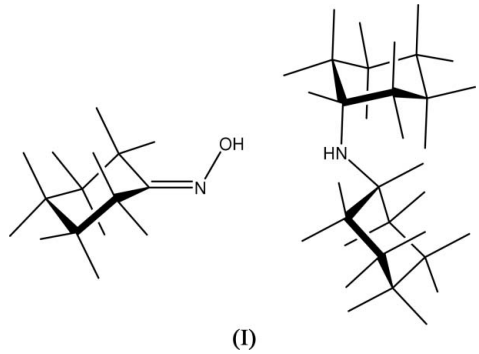
Comment

Both components of the title complex, (I) (Fig. 1), show the expected molecular geometries and both cyclohexane rings of the dicyclohexylamine molecule adopt the chair conformation. The conformation of the oxime six-membered ring is half-chair, very similar to that observed in the structure of cyclohexanone oxime itself (Olivato *et al.*, 2001). The geometrical parameters of the oxime fragment show standard values for oximes (Chertanova *et al.*,1994). The most interesting feature of this structure is the system of hydrogen bonds. The oxime hydrogen bonds were first classified by Bertolasi *et al.* (1982) and divided into three groups. The structures where the oxime unit is a donor group and forms one hydrogen bond are in group *A*. The structures with an additional hydrogen bond (oxime N atom is a hydrogen-bond acceptor) form group *B* and the structures with one more hydrogen bond, where the oxime O atom is the acceptor, are regarded as group *C*. The later and more elaborate classification introduced by Chertanova *et al.* (1994) shows very few examples of other motifs. In both cases the analyses did not include the directionality of the hydrogen bonds and supposed them to be in the plane of oxime group. In the case of complex (I), one of the two hydrogen bonds is the classical type *A* O—H···N bond (Table 1 and Fig. 2). However, the geometry of the second hydrogen bond cannot be regarded as a pure *B*- or *C*-type bond. The N—H vector is not in the plane of the oxime group and is pointed toward the centre of the oxime O—N bond of an adjacent molecule. Therefore, this can be classified as a weak bifurcated hydrogen bond and the overall resulting bonding of the oxime unit in complex (I) is intermediate between *B*- and *C*-types.



(I)

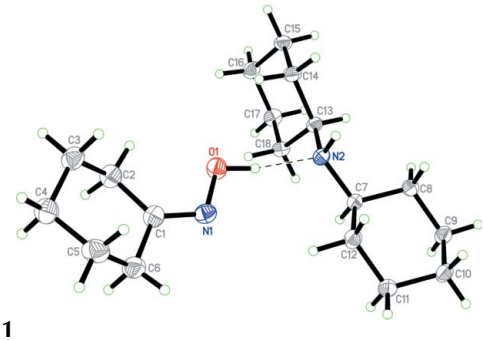


Figure 1
Structure of the molecular complex (I). Displacement ellipsoids are shown at the 50% probability level. The dashed line indicates a hydrogen bond.

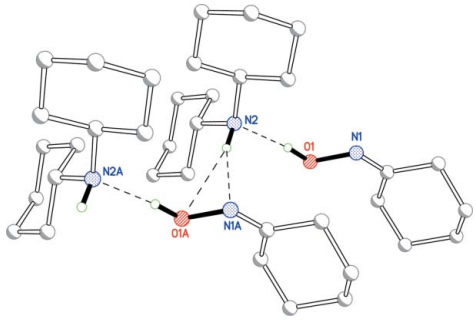


Figure 2
Hydrogen bonds (dashed lines) in the structure of (I). H atoms not involved in the interactions shown have been omitted.

The hydrogen bonds link the molecules into chains, parallel to the *c* axis. The oxime molecules in the chains are also connected by weak C1—H21···O1 (H···O = 2.71 Å) interactions. The chains form loose layers perpendicular to the *a* direction (Fig. 3)

Experimental

A solution of an organic compound (10 mg) in dicyclohexylamine (0.3 ml) was heated at 423 K in an open vessel for 2–3 min. The molecular complex (I) crystallized serendipitously as colourless needles after cooling of the solution, followed by standing at room temperature for several months. Presumably, the compound is a product of some oxidative conversion of the solvent.

Crystal data

$C_{12}H_{23}N{\cdot}C_6H_{11}NO$
M_r = 294.47
Orthorhombic, $Pna2_1$
a = 29.599 (6) Å
b = 11.359 (2) Å
c = 5.1586 (10) Å
V = 1734.3 (6) Å^3
Z = 4
D_x = 1.128 Mg m^{-3}
Mo- $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
Needle, colourless
0.70 × 0.04 × 0.03 mm

Data collection

Bruker SMART CCD 6000 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.953, T_{max} = 0.998
12334 measured reflections
2118 independent reflections
1714 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.0°

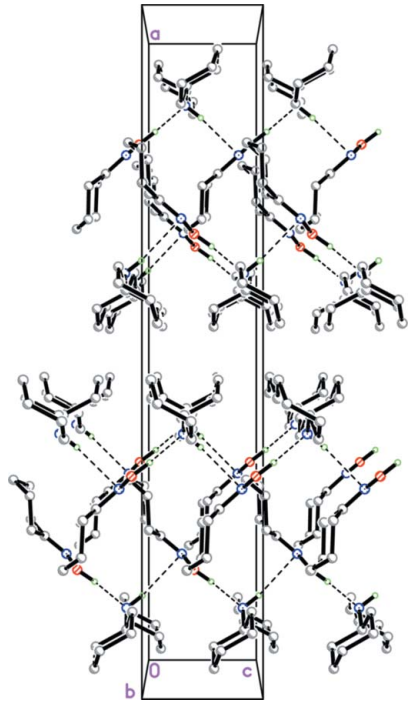


Figure 3
Packing of the molecules in the structure of (I), viewed along the *b* axis. H atoms not involved in the hydrogen bonds (dashed lines) shown have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.05
2118 reflections
326 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.419 (3)	N2—C13	1.477 (3)
N1—C1	1.292 (3)	N2—C7	1.484 (3)
C1—N1—O1	111.7 (2)	N2—C7—C8	113.1 (2)
C13—N2—C7	115.91 (16)	C12—C7—C8	110.0 (2)
N1—C1—C6	116.7 (2)	N2—C13—C18	111.0 (2)
N1—C1—C2	127.0 (2)	N2—C13—C14	108.67 (18)
C6—C1—C2	116.3 (2)	C18—C13—C14	109.7 (2)
N2—C7—C12	109.04 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···N2	0.98 (5)	1.85 (5)	2.818 (3)	167 (4)
N2—H2N···O1^{i}	0.90 (3)	2.62 (3)	3.509 (3)	167 (2)
N2—H2N···N1^{i}	0.90 (3)	2.59 (3)	3.451 (3)	160 (2)
C2—H21···O1^{ii}	1.04 (3)	2.71 (3)	3.686 (3)	155 (2)

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

All H atoms were located in a difference Fourier map and refined isotropically [C—H = 0.94 (3)–1.05 (4) Å].

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2003); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The manuscript was prepared with the beta test version 1.0.0. of the program *publCIF* to be released by the IUCr and with the program *modiCIFer* to be released by the University of Wisconsin–Madison.

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supporting information

Acta Cryst. (2006). E**62**, o2053–o2055 [https://doi.org/10.1107/S1600536806014310]

A 1:1 molecular complex of dicyclohexylamine and cyclohexanone oxime

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dicyclohexylamine–cyclohexanone oxime (1/1)

Crystal data

$C_{12}H_{23}N·C_6H_{11}NO$
M_r = 294.47
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
a = 29.599 (6) Å
b = 11.359 (2) Å
c = 5.1586 (10) Å
V = 1734.3 (6) Å^3
Z = 4
F(000) = 656
D_x = 1.128 Mg m^{-3}
Melting point: 58°C decomp. K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2345 reflections
θ = 2.3–25.1°
μ = 0.07 mm^{-1}
T = 120 K
Needle, colorless
0.70 × 0.04 × 0.03 mm

Data collection

Bruker SMART CCD 6000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
0.30° ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2003)
T_{min} = 0.953, T_{max} = 0.998
12334 measured reflections
2118 independent reflections
1714 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 27.0°, θ_{min} = 1.4°
h = −37→37
k = −13→14
l = −6→6

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.05
2118 reflections
326 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.03P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Special details

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

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.32558 (6)	0.20740 (15)	−0.0708 (4)	0.0284 (4)
N1	0.30521 (6)	0.10559 (17)	−0.1791 (5)	0.0261 (5)
N2	0.38448 (6)	0.16297 (17)	0.3470 (5)	0.0195 (4)
C1	0.27735 (8)	0.1321 (2)	−0.3629 (6)	0.0265 (6)
C2	0.26491 (8)	0.2533 (2)	−0.4549 (6)	0.0298 (6)
C3	0.21338 (8)	0.2667 (3)	−0.4673 (6)	0.0316 (6)
C4	0.19196 (8)	0.1679 (3)	−0.6259 (7)	0.0351 (7)
C5	0.20409 (9)	0.0486 (3)	−0.5094 (7)	0.0358 (7)
C6	0.25526 (9)	0.0314 (3)	−0.5012 (7)	0.0324 (6)
C7	0.41017 (8)	0.0510 (2)	0.3611 (5)	0.0188 (5)
C8	0.43432 (8)	0.0337 (2)	0.6211 (5)	0.0218 (5)
C9	0.45906 (8)	−0.0847 (2)	0.6313 (6)	0.0236 (5)
C10	0.42696 (9)	−0.1864 (2)	0.5793 (6)	0.0243 (5)
C11	0.40268 (9)	−0.1698 (2)	0.3212 (6)	0.0255 (6)
C12	0.37805 (8)	−0.0514 (2)	0.3108 (6)	0.0235 (5)
C13	0.41173 (7)	0.27190 (19)	0.3537 (5)	0.0188 (5)
C14	0.38047 (8)	0.3757 (2)	0.4116 (6)	0.0226 (5)
C15	0.40585 (8)	0.4933 (2)	0.4109 (5)	0.0237 (6)
C16	0.43019 (9)	0.5120 (2)	0.1532 (6)	0.0252 (6)
C17	0.46156 (8)	0.4084 (2)	0.0964 (6)	0.0244 (6)
C18	0.43562 (8)	0.2919 (2)	0.0967 (5)	0.0215 (5)
H1O	0.3443 (13)	0.180 (4)	0.074 (11)	0.094 (15)*
H2N	0.3656 (8)	0.167 (2)	0.484 (6)	0.014 (6)*
H21	0.2766 (11)	0.265 (3)	−0.644 (8)	0.052 (10)*
H22	0.2792 (9)	0.311 (2)	−0.338 (6)	0.031 (7)*
H31	0.2015 (10)	0.265 (3)	−0.276 (7)	0.037 (8)*
H32	0.2057 (9)	0.346 (2)	−0.539 (6)	0.032 (8)*
H41	0.1600 (9)	0.179 (2)	−0.621 (6)	0.030 (7)*
H42	0.2033 (11)	0.170 (3)	−0.814 (8)	0.050 (10)*
H51	0.1910 (9)	−0.014 (3)	−0.609 (6)	0.035 (8)*
H52	0.1931 (10)	0.043 (3)	−0.320 (7)	0.045 (9)*
H61	0.2671 (9)	0.032 (3)	−0.693 (7)	0.036 (8)*
H62	0.2613 (9)	−0.041 (3)	−0.420 (7)	0.041 (9)*
H7	0.4340 (8)	0.056 (2)	0.217 (6)	0.014 (6)*
H81	0.4567 (8)	0.097 (2)	0.652 (6)	0.026 (7)*
H82	0.4121 (9)	0.039 (2)	0.755 (6)	0.026 (8)*
H91	0.4727 (9)	−0.094 (2)	0.801 (7)	0.025 (7)*
H92	0.4848 (9)	−0.085 (2)	0.508 (6)	0.026 (7)*
H101	0.4425 (7)	−0.261 (2)	0.585 (6)	0.020 (6)*
H102	0.4043 (9)	−0.188 (2)	0.721 (6)	0.027 (7)*

H111	0.3807 (8)	−0.236 (2)	0.295 (6)	0.027 (7)*
H112	0.4229 (10)	−0.173 (3)	0.174 (7)	0.041 (9)*
H121	0.3541 (8)	−0.047 (2)	0.436 (6)	0.011 (6)*
H122	0.3618 (8)	−0.043 (2)	0.131 (6)	0.017 (6)*
H13	0.4362 (7)	0.272 (2)	0.488 (5)	0.013 (6)*
H141	0.3560 (8)	0.379 (2)	0.279 (6)	0.014 (6)*
H142	0.3664 (9)	0.361 (2)	0.574 (7)	0.029 (8)*
H151	0.4288 (8)	0.496 (2)	0.555 (6)	0.023 (7)*
H152	0.3842 (8)	0.562 (2)	0.446 (6)	0.025 (7)*
H161	0.4075 (8)	0.520 (2)	0.016 (6)	0.025 (7)*
H162	0.4466 (8)	0.587 (2)	0.161 (6)	0.030 (7)*
H171	0.4783 (9)	0.419 (2)	−0.064 (6)	0.023 (7)*
H172	0.4842 (10)	0.406 (2)	0.244 (7)	0.034 (8)*
H181	0.4111 (8)	0.292 (2)	−0.043 (6)	0.022 (7)*
H182	0.4567 (8)	0.228 (2)	0.065 (6)	0.021 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0275 (8)	0.0263 (8)	0.0313 (11)	−0.0048 (7)	−0.0057 (9)	0.0009 (8)
N1	0.0236 (9)	0.0232 (10)	0.0315 (12)	−0.0010 (8)	0.0008 (10)	−0.0015 (10)
N2	0.0184 (8)	0.0180 (9)	0.0221 (11)	0.0000 (8)	0.0005 (10)	0.0014 (8)
C1	0.0205 (10)	0.0295 (12)	0.0296 (15)	0.0005 (10)	0.0019 (11)	0.0012 (12)
C2	0.0239 (11)	0.0301 (13)	0.0355 (16)	−0.0034 (10)	−0.0017 (12)	0.0012 (13)
C3	0.0247 (12)	0.0322 (14)	0.0380 (17)	0.0040 (10)	−0.0018 (13)	−0.0003 (13)
C4	0.0208 (11)	0.0431 (15)	0.0414 (19)	0.0032 (12)	−0.0046 (14)	−0.0062 (13)
C5	0.0317 (14)	0.0314 (14)	0.044 (2)	−0.0061 (11)	−0.0032 (14)	−0.0082 (14)
C6	0.0312 (13)	0.0285 (14)	0.0376 (17)	0.0015 (11)	−0.0056 (13)	−0.0044 (13)
C7	0.0193 (10)	0.0174 (10)	0.0197 (13)	0.0011 (8)	0.0000 (10)	0.0016 (10)
C8	0.0229 (11)	0.0207 (11)	0.0218 (14)	0.0009 (9)	−0.0031 (11)	−0.0013 (11)
C9	0.0238 (12)	0.0203 (11)	0.0269 (15)	0.0008 (9)	−0.0053 (12)	0.0011 (11)
C10	0.0281 (12)	0.0180 (11)	0.0269 (14)	0.0007 (10)	−0.0035 (12)	0.0031 (11)
C11	0.0312 (12)	0.0195 (11)	0.0260 (15)	−0.0026 (10)	−0.0054 (13)	−0.0008 (12)
C12	0.0225 (11)	0.0212 (11)	0.0267 (13)	−0.0020 (9)	−0.0069 (13)	0.0014 (11)
C13	0.0190 (10)	0.0149 (11)	0.0224 (13)	0.0002 (8)	−0.0012 (10)	−0.0004 (10)
C14	0.0251 (11)	0.0195 (11)	0.0232 (13)	0.0029 (9)	0.0044 (11)	−0.0004 (11)
C15	0.0289 (12)	0.0175 (11)	0.0246 (14)	0.0005 (9)	0.0017 (12)	−0.0025 (11)
C16	0.0287 (12)	0.0190 (12)	0.0278 (14)	−0.0007 (10)	−0.0007 (12)	0.0029 (11)
C17	0.0229 (12)	0.0217 (12)	0.0286 (15)	−0.0039 (9)	0.0040 (12)	0.0025 (11)
C18	0.0207 (10)	0.0190 (11)	0.0247 (14)	0.0001 (9)	0.0029 (11)	−0.0021 (11)

Geometric parameters (Å, º)

O1—N1	1.419 (3)	C9—C10	1.519 (3)
O1—H1O	0.98 (5)	C9—H91	0.97 (3)
N1—C1	1.292 (3)	C9—H92	0.99 (3)
N2—C13	1.477 (3)	C10—C11	1.524 (4)
N2—C7	1.484 (3)	C10—H101	0.97 (3)

N2—H2N	0.90 (3)	C10—H102	0.99 (3)
C1—C6	1.499 (4)	C11—C12	1.530 (3)
C1—C2	1.503 (4)	C11—H111	1.00 (3)
C2—C3	1.534 (3)	C11—H112	0.97 (4)
C2—H21	1.04 (4)	C12—H121	0.96 (3)
C2—H22	0.98 (3)	C12—H122	1.05 (3)
C3—C4	1.527 (4)	C13—C18	1.520 (4)
C3—H31	1.05 (4)	C13—C14	1.528 (3)
C3—H32	1.00 (3)	C13—H13	1.00 (3)
C4—C5	1.525 (5)	C14—C15	1.532 (3)
C4—H41	0.95 (3)	C14—H141	1.00 (3)
C4—H42	1.03 (4)	C14—H142	0.95 (3)
C5—C6	1.528 (4)	C15—C16	1.527 (4)
C5—H51	0.96 (3)	C15—H151	1.01 (3)
C5—H52	1.03 (4)	C15—H152	1.03 (3)
C6—H61	1.05 (4)	C16—C17	1.528 (3)
C6—H62	0.94 (3)	C16—H161	0.98 (3)
C7—C12	1.525 (3)	C16—H162	0.98 (3)
C7—C8	1.532 (3)	C17—C18	1.529 (3)
C7—H7	1.03 (3)	C17—H171	0.97 (3)
C8—C9	1.532 (3)	C17—H172	1.01 (4)
C8—H81	0.99 (3)	C18—H181	1.02 (3)
C8—H82	0.96 (3)	C18—H182	0.97 (2)

N1—O1—H1O	106 (2)	H91—C9—H92	105 (2)
C1—N1—O1	111.7 (2)	C9—C10—C11	110.8 (2)
C13—N2—C7	115.91 (16)	C9—C10—H101	111.4 (14)
C13—N2—H2N	105.8 (15)	C11—C10—H101	111.0 (17)
C7—N2—H2N	109.1 (15)	C9—C10—H102	107.7 (16)
N1—C1—C6	116.7 (2)	C11—C10—H102	109.2 (17)
N1—C1—C2	127.0 (2)	H101—C10—H102	107 (2)
C6—C1—C2	116.3 (2)	C10—C11—C12	111.3 (2)
C1—C2—C3	110.3 (2)	C10—C11—H111	109.5 (17)
C1—C2—H21	109.2 (19)	C12—C11—H111	110.0 (14)
C3—C2—H21	106.1 (19)	C10—C11—H112	113.0 (19)
C1—C2—H22	108.2 (17)	C12—C11—H112	107.2 (18)
C3—C2—H22	112.7 (17)	H111—C11—H112	106 (2)
H21—C2—H22	110 (2)	C7—C12—C11	111.54 (19)
C4—C3—C2	111.2 (2)	C7—C12—H121	107.8 (14)
C4—C3—H31	110.5 (17)	C11—C12—H121	111.9 (14)
C2—C3—H31	107.0 (16)	C7—C12—H122	111.3 (13)
C4—C3—H32	111.8 (17)	C11—C12—H122	109.5 (14)
C2—C3—H32	109.3 (15)	H121—C12—H122	104.6 (19)
H31—C3—H32	107 (2)	N2—C13—C18	111.0 (2)
C5—C4—C3	110.1 (3)	N2—C13—C14	108.67 (18)
C5—C4—H41	109.8 (17)	C18—C13—C14	109.7 (2)
C3—C4—H41	107.5 (17)	N2—C13—H13	114.3 (14)
C5—C4—H42	108.4 (18)	C18—C13—H13	105.5 (14)

C3—C4—H42	110.8 (18)	C14—C13—H13	107.6 (14)
H41—C4—H42	110 (3)	C13—C14—C15	112.03 (19)
C4—C5—C6	111.0 (2)	C13—C14—H141	109.4 (14)
C4—C5—H51	110.5 (18)	C15—C14—H141	109.0 (14)
C6—C5—H51	108.7 (16)	C13—C14—H142	107.7 (17)
C4—C5—H52	110.8 (18)	C15—C14—H142	111.5 (17)
C6—C5—H52	106.2 (18)	H141—C14—H142	107 (2)
H51—C5—H52	109 (3)	C16—C15—C14	110.8 (2)
C1—C6—C5	110.4 (2)	C16—C15—H151	108.8 (16)
C1—C6—H61	107.6 (16)	C14—C15—H151	110.6 (15)
C5—C6—H61	107.7 (16)	C16—C15—H152	110.1 (17)
C1—C6—H62	112 (2)	C14—C15—H152	110.8 (13)
C5—C6—H62	108.2 (17)	H151—C15—H152	106 (2)
H61—C6—H62	111 (3)	C15—C16—C17	110.3 (2)
N2—C7—C12	109.04 (18)	C15—C16—H161	108.5 (16)
N2—C7—C8	113.1 (2)	C17—C16—H161	110.5 (16)
C12—C7—C8	110.0 (2)	C15—C16—H162	108.7 (19)
N2—C7—H7	105.8 (14)	C17—C16—H162	111.9 (15)
C12—C7—H7	110.2 (14)	H161—C16—H162	107 (2)
C8—C7—H7	108.7 (15)	C16—C17—C18	111.17 (19)
C9—C8—C7	111.4 (2)	C16—C17—H171	112.2 (16)
C9—C8—H81	108.3 (14)	C18—C17—H171	111.4 (16)
C7—C8—H81	111.0 (17)	C16—C17—H172	106.0 (17)
C9—C8—H82	111.2 (16)	C18—C17—H172	108.1 (17)
C7—C8—H82	107.7 (17)	H171—C17—H172	108 (2)
H81—C8—H82	107 (2)	C13—C18—C17	111.3 (2)
C10—C9—C8	111.2 (2)	C13—C18—H181	106.6 (15)
C10—C9—H91	109.9 (16)	C17—C18—H181	110.5 (14)
C8—C9—H91	108.8 (15)	C13—C18—H182	109.4 (16)
C10—C9—H92	111.2 (15)	C17—C18—H182	109.1 (14)
C8—C9—H92	110.6 (15)	H181—C18—H182	110 (2)

O1—N1—C1—C6	177.2 (2)	C8—C9—C10—C11	55.6 (3)
O1—N1—C1—C2	−2.2 (3)	C9—C10—C11—C12	−55.5 (3)
N1—C1—C2—C3	−129.7 (3)	N2—C7—C12—C11	179.7 (2)
C6—C1—C2—C3	50.8 (3)	C8—C7—C12—C11	−55.8 (3)
C1—C2—C3—C4	−52.8 (3)	C10—C11—C12—C7	56.2 (3)
C2—C3—C4—C5	58.0 (3)	C7—N2—C13—C18	74.5 (3)
C3—C4—C5—C6	−58.7 (3)	C7—N2—C13—C14	−164.8 (2)
N1—C1—C6—C5	129.0 (3)	N2—C13—C14—C15	−177.6 (2)
C2—C1—C6—C5	−51.5 (3)	C18—C13—C14—C15	−56.1 (3)
C4—C5—C6—C1	54.2 (4)	C13—C14—C15—C16	56.3 (3)
C13—N2—C7—C12	−171.5 (2)	C14—C15—C16—C17	−55.6 (3)
C13—N2—C7—C8	65.8 (3)	C15—C16—C17—C18	56.4 (3)
N2—C7—C8—C9	178.02 (19)	N2—C13—C18—C17	176.48 (18)
C12—C7—C8—C9	55.9 (3)	C14—C13—C18—C17	56.4 (3)
C7—C8—C9—C10	−56.3 (3)	C16—C17—C18—C13	−57.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···N2	0.98 (5)	1.85 (5)	2.818 (3)	167 (4)
N2—H2*N*···O1^{i}	0.90 (3)	2.62 (3)	3.509 (3)	167 (2)
N2—H2*N*···N1^{i}	0.90 (3)	2.59 (3)	3.451 (3)	160 (2)
C2—H21···O1^{ii}	1.04 (3)	2.71 (3)	3.686 (3)	155 (2)

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