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Carbamazepine *N*,*N*-dimethylformamide solvate

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.117
Data-to-parameter ratio = 15.1

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

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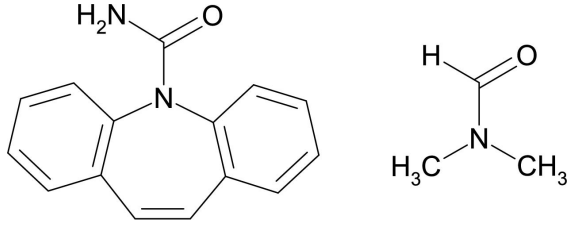
In the title compound, $C_{15}H_{12}N_2O\cdot C_3H_7NO$, carbamazepine molecules form the $R_2^2(8)$ N—H···O hydrogen-bonded dimer arrangement observed in the crystal structures of each of the four known anhydrous polymorphs. The molecules of *N*,*N*-dimethylformamide are located between adjacent carbamazepine dimers and form an N—H···O hydrogen bond to the *anti*-oriented NH group of the carboxamide moiety of carbamazepine.

Comment

The antiepileptic compound carbamazepine (CBZ) is known to crystallize in at least four anhydrous polymorphic forms (Grzesiak *et al.*, 2003) and the crystal structures of several solvates and co-crystals have also been reported (Fleischman *et al.*, 2003). The title solvate, (I), was produced during an automated parallel crystallization polymorph screen on CBZ. The sample was identified as a new form using multi-sample X-ray powder diffraction analysis of all recrystallized samples (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated *N*,*N*-dimethylformamide (DMF) solution by slow evaporation at 278 K yielded samples suitable for single-crystal X-ray analysis (Fig. 1).



(I)

In the crystal structure of (I), CBZ molecules form the centrosymmetric hydrogen-bonded $R_2^2(8)$ dimer motif observed in all of the known polymorphs and the majority of CBZ solvate crystal structures (Fleischman *et al.*, 2003) (Fig. 2). CBZ also forms a second N—H···O contact to atom O2 of the solvent molecule. Two C—H···O contacts exist between the DMF methyl H atoms (H17*C* and H18*B*) and atom O1 of CBZ. Atom O2 of DMF is further involved in a third C—H···O contact with an adjacent DMF molecule, forming a centrosymmetric $R_2^2(10)$ motif (Fig. 2). The CBZ dimers pack back-to-back, forming offset face-to-face hydrophobic interactions between adjacent azepine ring systems (Fig. 3).

Experimental

A single-crystal sample of the title compound was recrystallized from DMF solution by slow evaporation at 278 K.

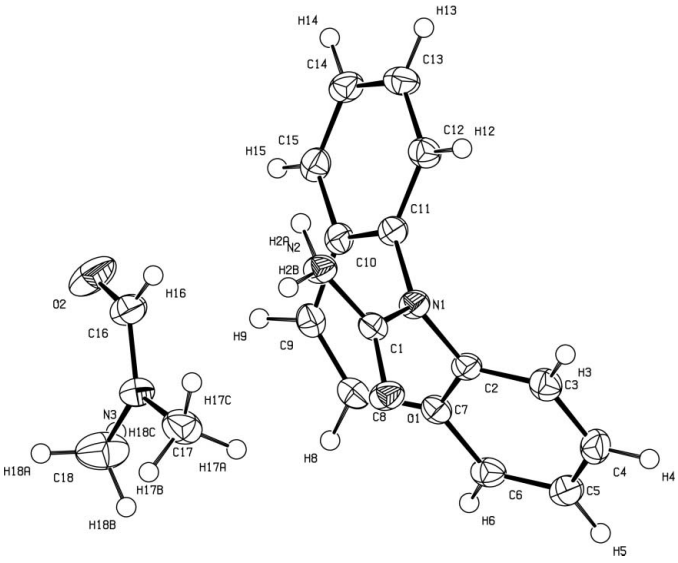


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids.

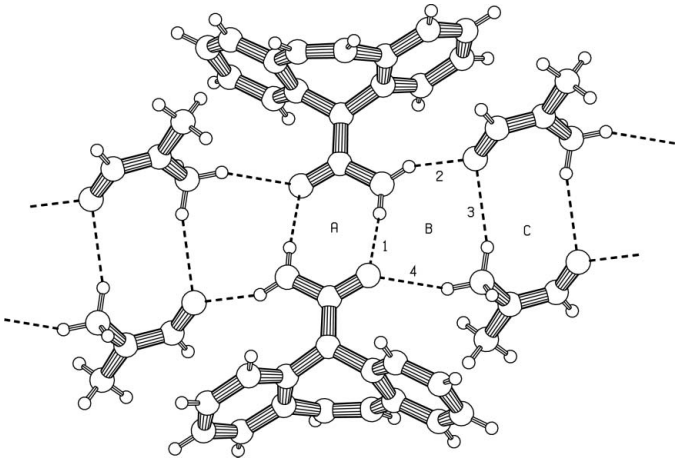


Figure 2
Packing diagram illustrating the non-covalent intermolecular network formed by (1) N2—H2*B*···O1 [N2···O1 = 2.9719 (19)Å O1 in the molecule at $2-x$, $-y$, $1-z$]; (2) N2—H2*A*···O2 [N2···O2 = 2.822 (2) Å; O2 in the molecule at $2-x$, $1-y$, $1-z$]; (3) C18—H18*C*···O2 [C18···O = 3.435 (3) Å; C18 in the molecule at $1+x$, *y*, *z*]; (4) C18—H18*B*···O1 [C18···O1 = 3.259 (2) Å; O1 in the molecule at $2-x$, $-y$, $1-z$] [calculated and illustrated using *PLATON* (Spek, 2003), program version 280604]. These interactions combine to produce three ring motifs: (A) the $R_2^2(8)$ CBZ dimer; (B) an $R_4^4(8)$ motif between CBZ dimers and molecules of DMF and (C) an $R_2^2(10)$ motif connecting DMF molecules in a centrosymmetric dimer configuration.

Crystal data

$C_{15}H_{12}N_2O{\cdot}C_3H_7NO$	$Z = 2$
$M_r = 309.36$	$D_x = 1.305$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.7118$ (4) Å	Cell parameters from 3432 reflections
$b = 9.1503$ (4) Å	$\theta = 2.9$–$27.0°$
$c = 11.6969$ (6) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 100.192$ (3)°	$T = 123$ (2) K
$\beta = 95.379$ (2)°	Fragment, colourless
$\gamma = 101.908$ (3)°	0.20 × 0.20 × 0.05 mm
$V = 787.58$ (7) Å^3	

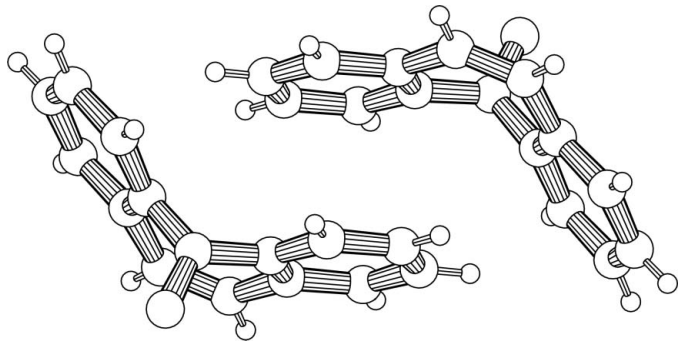


Figure 3
Hydrophobic packing interactions between nearest neighbour CBZ molecules with a centroid–centroid distance of 3.801 (1) Å (the carboxamide groups have been omitted for clarity).

Data collection

Nonius KappaCCD diffractometer	$R_{int} = 0.054$
ω and φ scans	$\theta_{max} = 27.2°$
Absorption correction: none	$h = -9 \rightarrow 9$
15107 measured reflections	$k = -11 \rightarrow 11$
3476 independent reflections	$l = -14 \rightarrow 14$
2475 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.208P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.048$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.117$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
3476 reflections	
230 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O2^{i}	0.921 (18)	1.963 (19)	2.822 (2)	154.5 (18)
N2—H2*B*···O1^{ii}	0.884 (19)	2.103 (19)	2.9719 (19)	167.4 (15)
C17—H17*C*···O1^{ii}	0.98	2.51	3.373 (3)	147
C18—H18*B*···O1^{iii}	0.98	2.43	3.259 (2)	142
C18—H18*C*···O2^{iv}	0.98	2.49	3.435 (3)	163

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

Five H atoms (H2*A*, H2*B*, H8, H9 and H16) were located in difference maps and refined isotropically, but all other H atoms were constrained to idealized geometry using a riding model; for CH_3 groups, $U_{iso}(H) = 1.5U_{eq}(C)$ and C—H = 0.98 Å, while for CH groups, $U_{iso}(H) = 1.2U_{eq}(C)$ and C—H = 0.95 Å.

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; 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: *SHELXL97*.

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Cell parameters from 3432 reflections
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Fragment, colourless
0.20 × 0.20 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
15107 measured reflections
3476 independent reflections
2475 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 27.2°$, $\theta_{min} = 3.1°$
$h = -9\rightarrow9$
$k = -11\rightarrow11$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.117$
$S = 1.03$
3476 reflections
230 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0505P)^2 + 0.208P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ 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	0.86234 (15)	−0.08670 (12)	0.35964 (10)	0.0275 (3)
O2	0.76776 (19)	0.54750 (14)	0.56447 (13)	0.0482 (4)
N1	0.84593 (17)	0.07785 (14)	0.23638 (11)	0.0228 (3)
N2	1.06578 (19)	0.13981 (17)	0.39877 (13)	0.0251 (3)
N3	0.68494 (19)	0.30325 (15)	0.58731 (13)	0.0269 (3)
C1	0.9231 (2)	0.03844 (18)	0.33519 (14)	0.0220 (3)
C2	0.6856 (2)	−0.02317 (17)	0.17131 (14)	0.0225 (4)
C3	0.6971 (2)	−0.15694 (19)	0.09830 (15)	0.0278 (4)
H3	0.8107	−0.1791	0.0895	0.033*
C4	0.5434 (2)	−0.2582 (2)	0.03832 (15)	0.0312 (4)
H4	0.5515	−0.3499	−0.0115	0.037*
C5	0.3778 (2)	−0.2257 (2)	0.05097 (15)	0.0302 (4)
H5	0.2721	−0.2951	0.0100	0.036*
C6	0.3666 (2)	−0.09263 (19)	0.12297 (15)	0.0277 (4)
H6	0.2523	−0.0715	0.1311	0.033*
C7	0.5203 (2)	0.01298 (18)	0.18488 (14)	0.0240 (4)
C8	0.5007 (2)	0.15180 (19)	0.26111 (15)	0.0263 (4)
C9	0.6154 (2)	0.28859 (19)	0.28799 (15)	0.0260 (4)
C10	0.7853 (2)	0.33202 (18)	0.24291 (14)	0.0242 (4)
C11	0.8920 (2)	0.22866 (18)	0.21166 (14)	0.0228 (4)
C12	1.0437 (2)	0.27058 (19)	0.15885 (15)	0.0261 (4)
H12	1.1135	0.1987	0.1366	0.031*
C13	1.0930 (2)	0.41757 (19)	0.13867 (15)	0.0296 (4)
H13	1.1958	0.4459	0.1017	0.036*
C14	0.9924 (2)	0.52293 (19)	0.17237 (15)	0.0295 (4)
H14	1.0276	0.6241	0.1600	0.035*
C15	0.8412 (2)	0.48080 (18)	0.22387 (14)	0.0269 (4)
H15	0.7733	0.5540	0.2470	0.032*
C16	0.7986 (3)	0.4210 (2)	0.56419 (16)	0.0332 (4)
C17	0.7293 (3)	0.1566 (2)	0.58202 (18)	0.0377 (5)
H17A	0.6608	0.0850	0.5123	0.057*
H17B	0.6997	0.1179	0.6524	0.057*
H17C	0.8575	0.1674	0.5777	0.057*
C18	0.5100 (3)	0.3173 (2)	0.6171 (2)	0.0510 (6)
H18A	0.5225	0.3760	0.6972	0.077*
H18B	0.4342	0.2155	0.6117	0.077*
H18C	0.4551	0.3698	0.5625	0.077*
H2B	1.102 (2)	0.1196 (19)	0.4670 (17)	0.024 (5)*
H2A	1.096 (3)	0.240 (2)	0.3909 (16)	0.038 (5)*
H16	0.917 (3)	0.399 (2)	0.5475 (18)	0.044 (6)*

H8	0.386 (2)	0.1441 (19)	0.2895 (15)	0.028 (5)*
H9	0.578 (2)	0.372 (2)	0.3334 (16)	0.029 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0302 (6)	0.0237 (6)	0.0275 (7)	0.0010 (5)	−0.0002 (5)	0.0107 (5)
O2	0.0570 (9)	0.0264 (7)	0.0524 (9)	−0.0058 (6)	−0.0159 (7)	0.0148 (6)
N1	0.0256 (7)	0.0214 (7)	0.0211 (7)	0.0033 (6)	0.0005 (6)	0.0075 (6)
N2	0.0263 (8)	0.0251 (8)	0.0233 (8)	0.0017 (6)	−0.0007 (6)	0.0107 (6)
N3	0.0253 (7)	0.0242 (7)	0.0313 (8)	0.0032 (6)	0.0038 (6)	0.0091 (6)
C1	0.0224 (8)	0.0233 (8)	0.0222 (9)	0.0064 (7)	0.0066 (7)	0.0063 (7)
C2	0.0263 (9)	0.0218 (8)	0.0189 (8)	0.0016 (7)	0.0010 (7)	0.0086 (6)
C3	0.0317 (10)	0.0290 (9)	0.0243 (9)	0.0073 (7)	0.0040 (7)	0.0087 (7)
C4	0.0436 (11)	0.0257 (9)	0.0222 (9)	0.0042 (8)	0.0024 (8)	0.0043 (7)
C5	0.0334 (10)	0.0304 (9)	0.0224 (9)	−0.0028 (8)	−0.0031 (7)	0.0094 (7)
C6	0.0252 (9)	0.0319 (9)	0.0258 (9)	0.0020 (7)	0.0014 (7)	0.0115 (7)
C7	0.0298 (9)	0.0252 (9)	0.0184 (8)	0.0041 (7)	0.0035 (7)	0.0100 (7)
C8	0.0256 (9)	0.0327 (10)	0.0231 (9)	0.0077 (8)	0.0063 (7)	0.0093 (7)
C9	0.0315 (9)	0.0270 (9)	0.0215 (9)	0.0100 (8)	0.0052 (7)	0.0055 (7)
C10	0.0284 (9)	0.0254 (9)	0.0171 (8)	0.0036 (7)	−0.0009 (7)	0.0051 (7)
C11	0.0262 (9)	0.0229 (8)	0.0184 (8)	0.0025 (7)	−0.0011 (7)	0.0073 (7)
C12	0.0270 (9)	0.0287 (9)	0.0235 (9)	0.0054 (7)	0.0032 (7)	0.0089 (7)
C13	0.0274 (9)	0.0329 (9)	0.0283 (9)	0.0004 (7)	0.0039 (7)	0.0126 (8)
C14	0.0363 (10)	0.0231 (9)	0.0273 (10)	0.0007 (7)	0.0004 (8)	0.0096 (7)
C15	0.0333 (10)	0.0232 (8)	0.0234 (9)	0.0063 (7)	0.0001 (7)	0.0046 (7)
C16	0.0366 (11)	0.0315 (10)	0.0260 (10)	−0.0053 (8)	−0.0045 (8)	0.0108 (8)
C17	0.0455 (12)	0.0310 (10)	0.0434 (12)	0.0129 (9)	0.0173 (9)	0.0151 (9)
C18	0.0340 (12)	0.0440 (12)	0.0823 (17)	0.0133 (10)	0.0153 (11)	0.0227 (12)

Geometric parameters (Å, º)

O1—C1	1.2379 (18)	C8—C9	1.341 (2)
O2—C16	1.228 (2)	C8—H8	0.964 (18)
N1—C1	1.388 (2)	C9—C10	1.464 (2)
N1—C2	1.437 (2)	C9—H9	0.960 (18)
N1—C11	1.4395 (19)	C10—C11	1.400 (2)
N2—C1	1.343 (2)	C10—C15	1.404 (2)
N2—H2B	0.884 (19)	C11—C12	1.390 (2)
N2—H2A	0.92 (2)	C12—C13	1.388 (2)
N3—C16	1.327 (2)	C12—H12	0.9500
N3—C17	1.444 (2)	C13—C14	1.385 (2)
N3—C18	1.449 (2)	C13—H13	0.9500
C2—C3	1.387 (2)	C14—C15	1.378 (2)
C2—C7	1.398 (2)	C14—H14	0.9500
C3—C4	1.384 (2)	C15—H15	0.9500
C3—H3	0.9500	C16—H16	1.01 (2)
C4—C5	1.385 (3)	C17—H17A	0.9800

C4—H4	0.9500	C17—H17B	0.9800
C5—C6	1.376 (2)	C17—H17C	0.9800
C5—H5	0.9500	C18—H18A	0.9800
C6—C7	1.408 (2)	C18—H18B	0.9800
C6—H6	0.9500	C18—H18C	0.9800
C7—C8	1.461 (2)		

C1—N1—C2	118.24 (13)	C10—C9—H9	114.5 (10)
C1—N1—C11	122.93 (13)	C11—C10—C15	117.76 (15)
C2—N1—C11	117.16 (12)	C11—C10—C9	122.68 (14)
C1—N2—H2B	115.4 (11)	C15—C10—C9	119.48 (15)
C1—N2—H2A	123.1 (12)	C12—C11—C10	120.85 (14)
H2B—N2—H2A	116.9 (16)	C12—C11—N1	119.50 (14)
C16—N3—C17	121.52 (16)	C10—C11—N1	119.64 (14)
C16—N3—C18	120.79 (16)	C13—C12—C11	119.94 (16)
C17—N3—C18	117.69 (15)	C13—C12—H12	120.0
O1—C1—N2	123.12 (15)	C11—C12—H12	120.0
O1—C1—N1	119.92 (14)	C14—C13—C12	120.07 (16)
N2—C1—N1	116.94 (14)	C14—C13—H13	120.0
C3—C2—C7	121.07 (15)	C12—C13—H13	120.0
C3—C2—N1	119.42 (15)	C15—C14—C13	119.90 (15)
C7—C2—N1	119.49 (14)	C15—C14—H14	120.0
C4—C3—C2	120.15 (16)	C13—C14—H14	120.0
C4—C3—H3	119.9	C14—C15—C10	121.41 (16)
C2—C3—H3	119.9	C14—C15—H15	119.3
C3—C4—C5	119.93 (16)	C10—C15—H15	119.3
C3—C4—H4	120.0	O2—C16—N3	124.8 (2)
C5—C4—H4	120.0	O2—C16—H16	121.5 (11)
C6—C5—C4	119.87 (16)	N3—C16—H16	113.7 (11)
C6—C5—H5	120.1	N3—C17—H17A	109.5
C4—C5—H5	120.1	N3—C17—H17B	109.5
C5—C6—C7	121.62 (16)	H17A—C17—H17B	109.5
C5—C6—H6	119.2	N3—C17—H17C	109.5
C7—C6—H6	119.2	H17A—C17—H17C	109.5
C2—C7—C6	117.35 (15)	H17B—C17—H17C	109.5
C2—C7—C8	123.25 (15)	N3—C18—H18A	109.5
C6—C7—C8	119.39 (15)	N3—C18—H18B	109.5
C9—C8—C7	127.99 (16)	H18A—C18—H18B	109.5
C9—C8—H8	117.3 (10)	N3—C18—H18C	109.5
C7—C8—H8	114.5 (10)	H18A—C18—H18C	109.5
C8—C9—C10	126.91 (16)	H18B—C18—H18C	109.5
C8—C9—H9	118.1 (10)		

C2—N1—C1—O1	5.9 (2)	C7—C8—C9—C10	2.6 (3)
C11—N1—C1—O1	170.75 (14)	C8—C9—C10—C11	−31.2 (3)
C2—N1—C1—N2	−175.61 (14)	C8—C9—C10—C15	145.31 (18)
C11—N1—C1—N2	−10.8 (2)	C15—C10—C11—C12	−2.8 (2)
C1—N1—C2—C3	−76.47 (19)	C9—C10—C11—C12	173.83 (15)

C11—N1—C2—C3	117.80 (16)	C15—C10—C11—N1	176.11 (14)
C1—N1—C2—C7	101.90 (17)	C9—C10—C11—N1	−7.3 (2)
C11—N1—C2—C7	−63.84 (19)	C1—N1—C11—C12	82.2 (2)
C7—C2—C3—C4	−0.7 (2)	C2—N1—C11—C12	−112.76 (17)
N1—C2—C3—C4	177.63 (14)	C1—N1—C11—C10	−96.67 (18)
C2—C3—C4—C5	0.2 (2)	C2—N1—C11—C10	68.34 (19)
C3—C4—C5—C6	0.1 (2)	C10—C11—C12—C13	1.3 (2)
C4—C5—C6—C7	0.1 (2)	N1—C11—C12—C13	−177.57 (15)
C3—C2—C7—C6	0.9 (2)	C11—C12—C13—C14	0.8 (2)
N1—C2—C7—C6	−177.44 (13)	C12—C13—C14—C15	−1.3 (3)
C3—C2—C7—C8	179.64 (15)	C13—C14—C15—C10	−0.2 (2)
N1—C2—C7—C8	1.3 (2)	C11—C10—C15—C14	2.3 (2)
C5—C6—C7—C2	−0.6 (2)	C9—C10—C15—C14	−174.47 (15)
C5—C6—C7—C8	−179.39 (15)	C17—N3—C16—O2	178.25 (17)
C2—C7—C8—C9	31.3 (3)	C18—N3—C16—O2	−0.8 (3)
C6—C7—C8—C9	−150.03 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.921 (18)	1.963 (19)	2.822 (2)	154.5 (18)
N2—H2*B*···O1^{ii}	0.884 (19)	2.103 (19)	2.9719 (19)	167.4 (15)
C17—H17*C*···O1^{ii}	0.98	2.51	3.373 (3)	147
C18—H18*B*···O1^{iii}	0.98	2.43	3.259 (2)	142
C18—H18*C*···O2^{iv}	0.98	2.49	3.435 (3)	163

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