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9*H*-Carbazole-9-carbaldehyde

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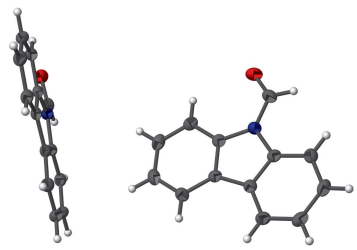
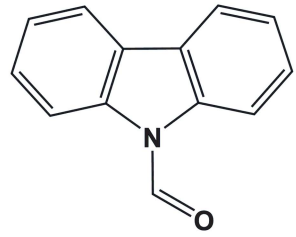
The title carbazole derivative, $C_{13}H_9NO$, crystallizes with two independent molecules (*A* and *B*) in the asymmetric unit. The dihedral angle between the planar carbazole ring system and the aldehyde group (HC═O) is 3.3 (2)° in *A* and 7.5 (2)° in *B*, indicating that the molecules are both nearly planar. In the crystal, the *A* and *B* molecules are linked by a C—H···O hydrogen bond and stack along the *b*-axis direction. The structure was refined as a two component twin with a refined BASF value of 0.102 (2).

3D view



Chemical scheme



Structure description

Carbazole derivatives are important compounds because of their wide range of biological activities, and also owing to their high electron affinity, hole transport properties and good planarity, which make them appropriate building blocks in the construction of chromophores for non-linear optical materials (Li *et al.* 2013; Jiang *et al.* 2016). Since carbazole derivatives have relatively low toxicity, they have been widely used in the biological area (Fei *et al.* 2015; Wang *et al.* 2016).

The title compound, Fig. 1, crystallized with two independent molecules (*A* and *B*) in the asymmetric unit. In molecule *A*, the aldehyde group (H13—C13═O1) is inclined to the planar carbazole ring system [N1/C1–C12; planar to within 0.019 (2) Å] by 3.3 (2)°. In molecule *B*, the aldehyde group (H27—C27═O2) is inclined to the planar carbazole ring system [N2/C15–C26; planar to within 0.014 (2) Å] by 7.5 (2)°. Hence, the two molecules are both almost planar. The geometrical parameters of the title compound are similar to those observed for 9-benzoylcarbazole (Claramunt *et al.*, 2002).

In the crystal, the *A* and *B* molecules are linked by a C—H···O hydrogen bond and stack along the *b*-axis direction (Table 1 and Fig. 2).

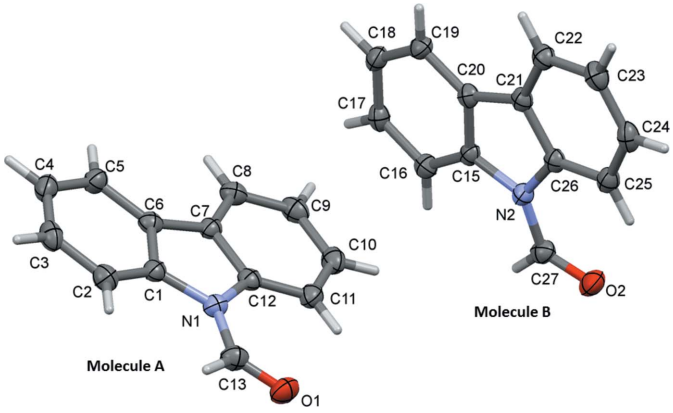


Figure 1
The molecular structure of the two independent molecules (*A* and *B*) of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

Synthesis and crystallization

The title compound was synthesized following a published procedure (Bose *et al.*, 2006). A mixture of 1.67 g (10.0 mmol) of carbazole and 1.0–1.2 equiv. of aqueous 80% formic acid in toluene was reacted for 10 min under microwave irradiation (320 W). The reaction was monitored by TLC, and after starting material had disappeared, the mixture was evaporated to give the crude title compound. Further purification by flash chromatography on silica gel, using petroleum ether/ethyl acetate (1:10 *v*/*v*) as eluent, gave a pale-yellow solid (yield 75%). The solid was then dissolved in 10 ml absolute ethanol, filtered, and the filtrate evaporated slowly for a week, yielding yellow rod-like crystals of the title compound. ^{1}H NMR (300 MHz, DMSO) δ 11.24 (*s*, 1H), 8.11 (*d*, *J* = 7.8 Hz, 2H), 7.48 (*d*, *J* = 8.1 Hz, 2H), 7.38 (*t*, *J* = 7.6 Hz, 2H), 7.15 (*t*, *J* = 7.4 Hz, 2H).

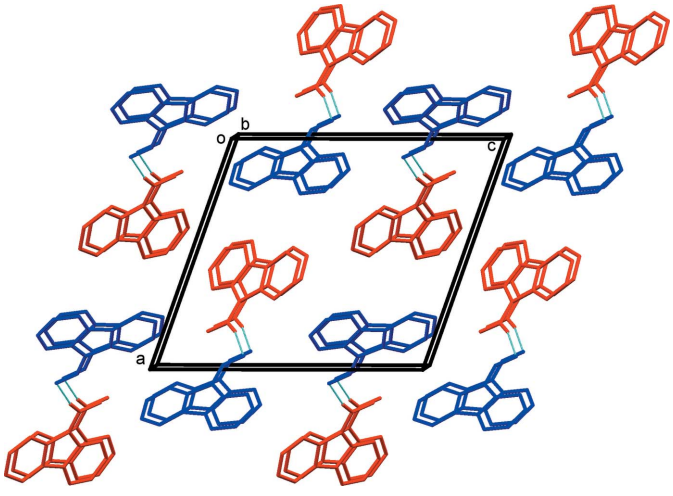


Figure 2
A view along the *b* axis of the crystal packing of the title compound. The *A* (blue) and *B* (red) molecules are linked by a C—H···O hydrogen bond and stack along the *b*-axis direction (see Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C27—H27···O1^{i}	0.93	2.47	3.378 (3)	166

Symmetry code: (i) $-x, y-\frac{3}{2}, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_9NO$
M_r	195.21
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	296
a, *b*, *c* (Å)	12.957 (2), 5.3621 (10), 14.440 (3)
β (°)	109.548 (2)
V (Å^3)	945.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker SMART CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.974, 0.983
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3577, 3577, 3457
R_{int}	0.018
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.644
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.029, 0.076, 1.07
No. of reflections	3577
No. of parameters	273
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.16

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010)'.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component twin with a refined BASF value of 0.102 (2).

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161757 [https://doi.org/10.1107/S2414314616017570]

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Crystal data

$C_{13}H_9NO$
M_r = 195.21
Monoclinic, $P2_1$
a = 12.957 (2) Å
b = 5.3621 (10) Å
c = 14.440 (3) Å
β = 109.548 (2)°
V = 945.4 (3) Å^3
Z = 4
$F(000)$ = 408
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5371 reflections
θ = 2.6–27.0°
μ = 0.09 mm^{-1}
T = 296 K
Rod, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.974, T_{max} = 0.983
3577 measured reflections
3577 independent reflections
3457 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 27.2°, θ_{min} = 1.5°
h = −16→16
k = −6→6
l = −15→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.076
S = 1.07
3577 reflections
273 parameters
1 restraint
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.1094P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.011 (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.

Refinement. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.07452 (11)	1.2319 (3)	0.34069 (11)	0.0349 (4)
N1	0.04534 (12)	1.0956 (3)	0.26573 (11)	0.0241 (3)
C1	0.08756 (14)	1.1098 (4)	0.18707 (13)	0.0238 (4)
C2	0.06519 (16)	1.2822 (4)	0.11060 (14)	0.0290 (4)
H2	0.0155	1.4113	0.1048	0.035*
C3	0.11964 (17)	1.2538 (4)	0.04364 (14)	0.0321 (5)
H3	0.1060	1.3655	−0.0084	0.038*
C4	0.19488 (16)	1.0603 (5)	0.05256 (14)	0.0319 (5)
H4	0.2305	1.0458	0.0066	0.038*
C5	0.21699 (15)	0.8901 (4)	0.12896 (14)	0.0283 (4)
H5	0.2670	0.7617	0.1346	0.034*
C6	0.16291 (15)	0.9149 (4)	0.19725 (14)	0.0236 (4)
C7	0.16787 (14)	0.7763 (4)	0.28531 (13)	0.0223 (4)
C8	0.22834 (15)	0.5698 (4)	0.33153 (14)	0.0274 (4)
H8	0.2761	0.4913	0.3051	0.033*
C9	0.21617 (16)	0.4829 (4)	0.41779 (15)	0.0308 (5)
H9	0.2561	0.3450	0.4494	0.037*
C10	0.14431 (16)	0.6008 (5)	0.45775 (14)	0.0313 (5)
H10	0.1377	0.5400	0.5158	0.038*
C11	0.08271 (15)	0.8061 (4)	0.41284 (14)	0.0281 (4)
H11	0.0349	0.8836	0.4396	0.034*
C12	0.09520 (15)	0.8919 (4)	0.32609 (14)	0.0236 (4)
C13	−0.03400 (16)	1.2500 (4)	0.27651 (15)	0.0296 (4)
H13	−0.0587	1.3785	0.2312	0.036*
O2	0.16975 (11)	0.3158 (3)	0.83309 (10)	0.0329 (4)
N2	0.29786 (12)	0.3523 (3)	0.75651 (11)	0.0226 (4)
C15	0.34916 (14)	0.2512 (4)	0.69175 (12)	0.0212 (4)
C16	0.31665 (15)	0.0519 (4)	0.62757 (13)	0.0241 (4)
H16	0.2526	−0.0358	0.6206	0.029*
C17	0.38418 (16)	−0.0113 (4)	0.57397 (14)	0.0262 (4)
H17	0.3648	−0.1440	0.5301	0.031*
C18	0.48043 (15)	0.1204 (4)	0.58462 (14)	0.0268 (4)
H18	0.5244	0.0732	0.5482	0.032*
C19	0.51149 (15)	0.3209 (4)	0.64885 (14)	0.0257 (4)
H19	0.5753	0.4092	0.6553	0.031*
C20	0.44523 (14)	0.3873 (4)	0.70346 (13)	0.0216 (4)
C21	0.45419 (14)	0.5768 (4)	0.77753 (13)	0.0225 (4)
C22	0.53065 (15)	0.7648 (4)	0.81761 (13)	0.0258 (4)
H22	0.5916	0.7835	0.7979	0.031*
C23	0.51438 (17)	0.9228 (4)	0.88710 (14)	0.0300 (4)
H23	0.5648	1.0488	0.9142	0.036*
C24	0.42294 (17)	0.8954 (4)	0.91706 (14)	0.0295 (4)
H24	0.4138	1.0039	0.9640	0.035*
C25	0.34560 (16)	0.7107 (4)	0.87868 (14)	0.0266 (4)
H25	0.2848	0.6934	0.8987	0.032*

C26	0.36272 (15)	0.5518 (4)	0.80878 (13)	0.0218 (4)
C27	0.20807 (15)	0.2484 (4)	0.77125 (14)	0.0264 (4)
H27	0.1739	0.1164	0.7308	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0335 (7)	0.0374 (9)	0.0392 (8)	0.0030 (7)	0.0195 (6)	−0.0046 (7)
N1	0.0228 (7)	0.0241 (9)	0.0265 (8)	−0.0001 (7)	0.0097 (6)	−0.0009 (7)
C1	0.0213 (8)	0.0260 (10)	0.0237 (9)	−0.0040 (8)	0.0072 (7)	−0.0048 (8)
C2	0.0304 (10)	0.0264 (11)	0.0283 (10)	−0.0004 (9)	0.0071 (8)	−0.0005 (9)
C3	0.0385 (11)	0.0324 (12)	0.0229 (10)	−0.0069 (10)	0.0071 (8)	0.0030 (9)
C4	0.0333 (10)	0.0398 (13)	0.0252 (10)	−0.0057 (10)	0.0131 (8)	−0.0043 (9)
C5	0.0267 (10)	0.0316 (11)	0.0284 (10)	0.0009 (9)	0.0116 (8)	−0.0032 (9)
C6	0.0213 (9)	0.0227 (10)	0.0251 (9)	−0.0025 (7)	0.0055 (7)	−0.0028 (8)
C7	0.0205 (8)	0.0234 (10)	0.0233 (9)	−0.0034 (8)	0.0078 (7)	−0.0038 (8)
C8	0.0242 (9)	0.0257 (11)	0.0310 (10)	0.0008 (8)	0.0073 (8)	−0.0004 (9)
C9	0.0287 (10)	0.0276 (11)	0.0316 (10)	−0.0002 (8)	0.0041 (8)	0.0053 (9)
C10	0.0315 (10)	0.0371 (12)	0.0243 (9)	−0.0084 (10)	0.0079 (8)	0.0032 (9)
C11	0.0268 (9)	0.0333 (11)	0.0259 (9)	−0.0052 (9)	0.0109 (8)	−0.0031 (8)
C12	0.0210 (8)	0.0238 (10)	0.0249 (9)	−0.0042 (8)	0.0062 (7)	−0.0029 (8)
C13	0.0271 (9)	0.0267 (11)	0.0347 (11)	0.0029 (8)	0.0100 (8)	−0.0027 (9)
O2	0.0333 (7)	0.0396 (10)	0.0322 (7)	0.0029 (7)	0.0194 (6)	0.0050 (7)
N2	0.0239 (8)	0.0236 (9)	0.0222 (8)	0.0019 (6)	0.0103 (6)	0.0011 (6)
C15	0.0233 (8)	0.0219 (10)	0.0195 (8)	0.0043 (8)	0.0087 (7)	0.0049 (8)
C16	0.0249 (9)	0.0228 (10)	0.0240 (9)	−0.0013 (8)	0.0073 (7)	0.0026 (8)
C17	0.0340 (10)	0.0233 (10)	0.0204 (9)	0.0020 (8)	0.0080 (8)	−0.0015 (8)
C18	0.0298 (9)	0.0305 (11)	0.0238 (9)	0.0036 (8)	0.0139 (8)	0.0014 (8)
C19	0.0240 (9)	0.0298 (11)	0.0256 (9)	−0.0001 (8)	0.0112 (8)	0.0030 (8)
C20	0.0249 (9)	0.0190 (9)	0.0206 (9)	0.0010 (7)	0.0071 (7)	0.0039 (8)
C21	0.0254 (9)	0.0216 (10)	0.0201 (8)	0.0031 (8)	0.0071 (7)	0.0045 (8)
C22	0.0278 (9)	0.0257 (11)	0.0233 (9)	−0.0016 (8)	0.0076 (7)	0.0035 (8)
C23	0.0353 (11)	0.0253 (11)	0.0260 (10)	−0.0018 (9)	0.0059 (8)	0.0009 (8)
C24	0.0398 (11)	0.0260 (11)	0.0209 (9)	0.0051 (9)	0.0079 (8)	−0.0012 (8)
C25	0.0299 (9)	0.0273 (11)	0.0239 (9)	0.0063 (8)	0.0109 (8)	0.0032 (8)
C26	0.0246 (9)	0.0207 (10)	0.0194 (8)	0.0031 (7)	0.0063 (7)	0.0043 (7)
C27	0.0246 (9)	0.0282 (11)	0.0278 (9)	0.0007 (8)	0.0106 (8)	0.0070 (8)

Geometric parameters (Å, º)

O1—C13	1.212 (2)	O2—C27	1.213 (2)
N1—C13	1.369 (3)	N2—C27	1.369 (2)
N1—C12	1.412 (3)	N2—C26	1.413 (2)
N1—C1	1.418 (2)	N2—C15	1.423 (2)
C1—C2	1.394 (3)	C15—C16	1.385 (3)
C1—C6	1.404 (3)	C15—C20	1.403 (3)
C2—C3	1.383 (3)	C16—C17	1.390 (3)
C2—H2	0.9300	C16—H16	0.9300

C3—C4	1.400 (3)	C17—C18	1.396 (3)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.386 (3)	C18—C19	1.389 (3)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.394 (3)	C19—C20	1.392 (3)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.456 (3)	C20—C21	1.452 (3)
C7—C8	1.391 (3)	C21—C22	1.396 (3)
C7—C12	1.410 (2)	C21—C26	1.409 (2)
C8—C9	1.387 (3)	C22—C23	1.382 (3)
C8—H8	0.9300	C22—H22	0.9300
C9—C10	1.400 (3)	C23—C24	1.398 (3)
C9—H9	0.9300	C23—H23	0.9300
C10—C11	1.387 (3)	C24—C25	1.386 (3)
C10—H10	0.9300	C24—H24	0.9300
C11—C12	1.394 (3)	C25—C26	1.394 (3)
C11—H11	0.9300	C25—H25	0.9300
C13—H13	0.9300	C27—H27	0.9300

C13—N1—C12	127.14 (16)	C27—N2—C26	127.54 (16)
C13—N1—C1	124.34 (17)	C27—N2—C15	123.73 (18)
C12—N1—C1	108.47 (15)	C26—N2—C15	108.31 (15)
C2—C1—C6	121.97 (17)	C16—C15—C20	122.73 (16)
C2—C1—N1	129.53 (18)	C16—C15—N2	128.99 (17)
C6—C1—N1	108.48 (17)	C20—C15—N2	108.27 (16)
C3—C2—C1	117.48 (19)	C15—C16—C17	116.96 (17)
C3—C2—H2	121.3	C15—C16—H16	121.5
C1—C2—H2	121.3	C17—C16—H16	121.5
C2—C3—C4	121.31 (19)	C16—C17—C18	121.40 (18)
C2—C3—H3	119.3	C16—C17—H17	119.3
C4—C3—H3	119.3	C18—C17—H17	119.3
C5—C4—C3	120.90 (18)	C19—C18—C17	120.91 (17)
C5—C4—H4	119.6	C19—C18—H18	119.5
C3—C4—H4	119.6	C17—C18—H18	119.5
C4—C5—C6	118.78 (19)	C18—C19—C20	118.70 (18)
C4—C5—H5	120.6	C18—C19—H19	120.6
C6—C5—H5	120.6	C20—C19—H19	120.6
C5—C6—C1	119.56 (18)	C19—C20—C15	119.29 (18)
C5—C6—C7	133.13 (19)	C19—C20—C21	133.13 (18)
C1—C6—C7	107.31 (16)	C15—C20—C21	107.56 (15)
C8—C7—C12	119.81 (18)	C22—C21—C26	119.50 (17)
C8—C7—C6	132.74 (17)	C22—C21—C20	132.98 (16)
C12—C7—C6	107.44 (17)	C26—C21—C20	107.51 (16)
C9—C8—C7	118.89 (18)	C23—C22—C21	118.95 (17)
C9—C8—H8	120.6	C23—C22—H22	120.5
C7—C8—H8	120.6	C21—C22—H22	120.5
C8—C9—C10	120.6 (2)	C22—C23—C24	120.72 (19)
C8—C9—H9	119.7	C22—C23—H23	119.6

C10—C9—H9	119.7	C24—C23—H23	119.6
C11—C10—C9	121.61 (19)	C25—C24—C23	121.72 (19)
C11—C10—H10	119.2	C25—C24—H24	119.1
C9—C10—H10	119.2	C23—C24—H24	119.1
C10—C11—C12	117.41 (19)	C24—C25—C26	117.21 (18)
C10—C11—H11	121.3	C24—C25—H25	121.4
C12—C11—H11	121.3	C26—C25—H25	121.4
C11—C12—C7	121.65 (19)	C25—C26—C21	121.91 (18)
C11—C12—N1	130.04 (18)	C25—C26—N2	129.73 (17)
C7—C12—N1	108.30 (16)	C21—C26—N2	108.35 (15)
O1—C13—N1	124.9 (2)	O2—C27—N2	124.9 (2)
O1—C13—H13	117.6	O2—C27—H27	117.6
N1—C13—H13	117.6	N2—C27—H27	117.6

C13—N1—C1—C2	4.3 (3)	C27—N2—C15—C16	5.7 (3)
C12—N1—C1—C2	−178.30 (19)	C26—N2—C15—C16	178.78 (18)
C13—N1—C1—C6	−176.87 (18)	C27—N2—C15—C20	−173.23 (16)
C12—N1—C1—C6	0.5 (2)	C26—N2—C15—C20	−0.1 (2)
C6—C1—C2—C3	0.5 (3)	C20—C15—C16—C17	0.2 (3)
N1—C1—C2—C3	179.17 (19)	N2—C15—C16—C17	−178.55 (18)
C1—C2—C3—C4	−0.4 (3)	C15—C16—C17—C18	0.1 (3)
C2—C3—C4—C5	0.2 (3)	C16—C17—C18—C19	−0.5 (3)
C3—C4—C5—C6	−0.1 (3)	C17—C18—C19—C20	0.6 (3)
C4—C5—C6—C1	0.2 (3)	C18—C19—C20—C15	−0.3 (3)
C4—C5—C6—C7	−178.6 (2)	C18—C19—C20—C21	177.9 (2)
C2—C1—C6—C5	−0.4 (3)	C16—C15—C20—C19	−0.1 (3)
N1—C1—C6—C5	−179.32 (17)	N2—C15—C20—C19	178.90 (16)
C2—C1—C6—C7	178.65 (17)	C16—C15—C20—C21	−178.76 (17)
N1—C1—C6—C7	−0.3 (2)	N2—C15—C20—C21	0.2 (2)
C5—C6—C7—C8	−0.3 (4)	C19—C20—C21—C22	2.6 (4)
C1—C6—C7—C8	−179.1 (2)	C15—C20—C21—C22	−179.0 (2)
C5—C6—C7—C12	178.8 (2)	C19—C20—C21—C26	−178.7 (2)
C1—C6—C7—C12	−0.1 (2)	C15—C20—C21—C26	−0.2 (2)
C12—C7—C8—C9	−0.5 (3)	C26—C21—C22—C23	−0.2 (3)
C6—C7—C8—C9	178.5 (2)	C20—C21—C22—C23	178.5 (2)
C7—C8—C9—C10	0.0 (3)	C21—C22—C23—C24	0.0 (3)
C8—C9—C10—C11	0.4 (3)	C22—C23—C24—C25	−0.1 (3)
C9—C10—C11—C12	−0.2 (3)	C23—C24—C25—C26	0.2 (3)
C10—C11—C12—C7	−0.3 (3)	C24—C25—C26—C21	−0.3 (3)
C10—C11—C12—N1	−179.03 (19)	C24—C25—C26—N2	−178.85 (18)
C8—C7—C12—C11	0.6 (3)	C22—C21—C26—C25	0.3 (3)
C6—C7—C12—C11	−178.60 (18)	C20—C21—C26—C25	−178.64 (17)
C8—C7—C12—N1	179.61 (16)	C22—C21—C26—N2	179.13 (16)
C6—C7—C12—N1	0.4 (2)	C20—C21—C26—N2	0.2 (2)
C13—N1—C12—C11	−4.4 (3)	C27—N2—C26—C25	−8.6 (3)
C1—N1—C12—C11	178.3 (2)	C15—N2—C26—C25	178.65 (18)
C13—N1—C12—C7	176.75 (18)	C27—N2—C26—C21	172.73 (18)
C1—N1—C12—C7	−0.6 (2)	C15—N2—C26—C21	0.0 (2)

C12—N1—C13—O1	−0.7 (3)	C26—N2—C27—O2	0.3 (3)
C1—N1—C13—O1	176.17 (19)	C15—N2—C27—O2	172.09 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C27—H27···O1^{i}	0.93	2.47	3.378 (3)	166

Symmetry code: (i) −*x*, *y*−3/2, −*z*+1.