IUCrData

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N,*N*-Dibutyl-4-[(*E*)-2-(2,5-dicyano-4-{(*E*)-2-[4-(dibutylamino)phenyl]ethenyl}phenyl)ethenyl]aniline

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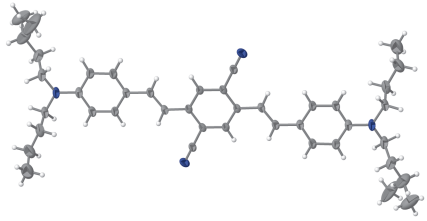
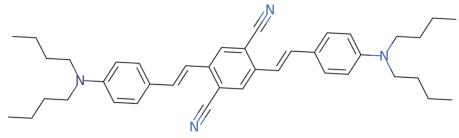
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{40}H_{50}N_4$, has been prepared *via* Horner olefination. The molecule is located on a centre of inversion with half a molecule in the asymmetric unit. The π-system is essentially planar and the molecules are arranged in layers separated by alkyl chains. As all cyano groups interact with neighbouring amino groups, a pattern composed of alternating orthogonal molecules results.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) is a linear *para*-distyrylbenzene with a donor–acceptor–donor (*DAD*) electronic structure (Pond *et al.*, 2002). It was prepared in a project on phenylenevinylene dyes (Stalmach & Detert, 2000) with focus on increased two-photon absorption (Detert *et al.*, 2004; Detert *et al.*, 2006; Strehmel *et al.*, 2003) and acidochromic fluorophors (Moschel *et al.*, 2026; Schmitt *et al.*, 2013). The electronic structure had been studied (Nemkovich *et al.*, 2010) and two-photon absorption has been investigated (Sumalekshmy & Fahrni, 2011). The crystal structures of two related cyanodistyrylbenzenes have been reported and both compounds crystallize centrosymmetrically (Mamada *et al.*, 2021). In the crystal of the title compound, the molecule is centrosymmetric, the π-system is essentially planar and the alkyl chains are disordered. At atom C20, two split positions could be refined [s.o.f. = 0.876 (10)/0.124 C20/C20*A*]. The torsion angle between the central ring and the vinylene group C2—C3—C4—C5 is −173.47 (19)° and the vinylene group C3—C4—C5—C6 and the terminal ring subtend an angle of 176.55 (18)°; the dihedral angle between the planes of the central and terminal rings is 2.40 (8)°. The angle sum at the aniline N atom is 358.89°, with the N atom being 0.0801 (16) Å above the C9/N12/C13/C17 plane. In the extended structure, the molecules are arranged in layers parallel to a diagonal of the unit cell. Butyl chains provoke the distance of the conjugated segments. Within the layer, a pattern composed of orthogonal molecules is formed. When looking along the *a*-axis direction, the molecules are rotated about 90° (Fig. 2). Every cyano N atom has a distance of 4.095 (2) Å to the next aniline N

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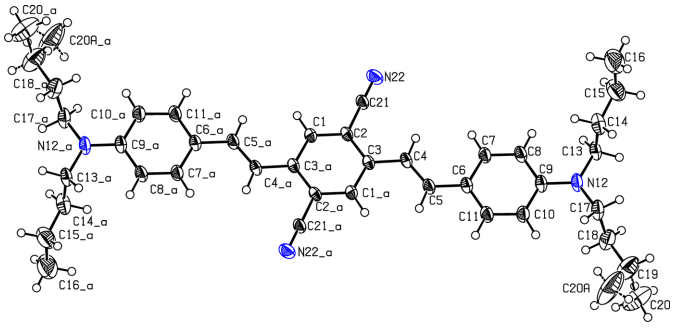

Figure 1
View of the title compound, with displacement ellipsoids drawn at the 50% probability level.

atom and this N···N≡C relation is nearly linear [174.11 (9)°]. Planarity and the cyano–amine interaction imply a high level of conjugation in this octupolar dye.

Synthesis and crystallization

The title compound was obtained in a Horner olefination of 1,4-bis(diethoxyphosphorylmethyl)-2,5-dicyanobenzene and 4-(dibutylamino)benzaldehyde in tetrahydrofuran (THF) using KOtBu as a base in 67% yield (Detert *et al.*, 2006). Recrystallization from a solvent mixture of 2-propanol and chloroform by slow evaporation yielded red needles (m.p. 447 K). Annotation of NMR signals follows IUPAC nomenclature. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (*s*, 2H, ph-CN), 7.43 (*d*, J = 8 Hz, 4H, 3-H, 5-H ph), 7.18 (*d*, J = 15 Hz, 2H, vin), 7.16 (*d*, J = 15 Hz, 2H, vin), 6.61 (*d*, J = 8 Hz, 4H, 2-H, 6-H ph), 3.32 (*t*, 8H, N—CH_2), 1.63 (*q*, 8H, β-CH_2), 1.38 (*q*, 8H, CH_2), 0.96 (*t*, 12, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.32 (N—C-4; 139.00, 134.86, (C_q), 129.40 (C-2, C-6 ph), 129.28, 123.12, 117.70, 114.37 (C_q, H-phCN), 111.96 (C-3, C-5 ph), 51.23 (N—CH_2), 29.89, 20.77 (CH_2), 14.45 (CH_3).

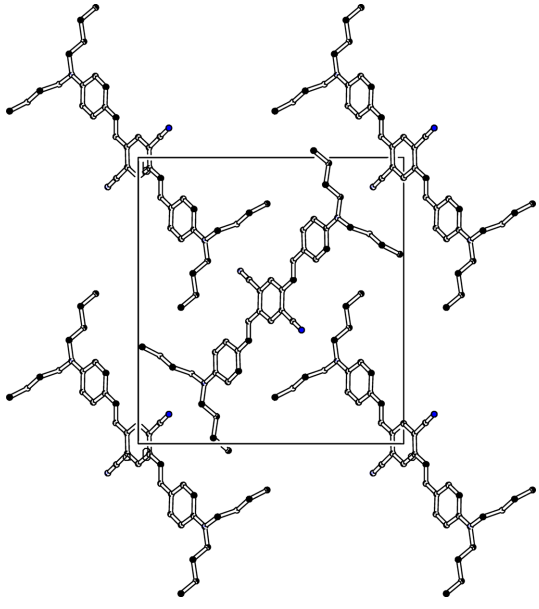

Figure 2
Part of the packing diagram, viewed along *a*-axis direction. H atoms and disordered atom C20*A* have been omitted for clarity.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{40}H_{50}N_4$
M_r	586.84
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	120
a, b, c (Å)	5.1999 (4), 19.7775 (11), 18.3877 (15)
β (°)	94.421 (6)
V (Å^3)	1885.4 (2)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.06
Crystal size (mm)	0.29 × 0.13 × 0.06
Data collection	
Diffractometer	STOE STADIVARI
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11216, 4326, 2874
R_{int}	0.053
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.071, 0.226, 1.04
No. of reflections	4326
No. of parameters	212
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.28

Computer programs: *WINXPOSE* in *X-AREA* (Stoe & Cie, 2020), *RECIPE* in *X-AREA* (Stoe & Cie, 2020), *INTEGRATE* in *X-AREA* (Stoe & Cie, 2020), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2019* (Sheldrick, 2015*b*) and *PLATON* (Spek, 2020).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed at calculated positions and were refined in the riding-model approximation, with aromatic C—H = 0.95 Å, methylene C—H = 0.99 Å and methyl C—H = 0.98 Å, and with U_{iso}(H) = 1.5U_{eq}(methyl C) and 1.2U_{eq}(C) for the remaining H atoms. The methyl groups were allowed to rotate but not to tip.

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full crystallographic data

IUCrData (2026). **11**, x261207 [https://doi.org/10.1107/S2414314626012071]

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_N_,_N_-Dibutyl-4-[(_E_)-2-(2,5-dicyano-4-{(_E_)-2-[4-(dibutylamino)phenyl]ethenyl}phenyl)ethenyl]aniline

Crystal data

$C_{40}H_{50}N_4$
M_r = 586.84
Monoclinic, $P2_1/c$
a = 5.1999 (4) Å
b = 19.7775 (11) Å
c = 18.3877 (15) Å
β = 94.421 (6)°
V = 1885.4 (2) Å^3
Z = 2
$F(000)$ = 636
D_x = 1.034 Mg m^{-3}
Melting point: 447 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10217 reflections
θ = 2.2–34.0°
μ = 0.06 mm^{-1}
T = 120 K
Block, brown
0.29 × 0.13 × 0.06 mm

Data collection

STOE STADIVARI diffractometer
Radiation source: Axo Mo
Detector resolution: 13.33 pixels mm^{-1}
rotation method, ω scans
11216 measured reflections
4326 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −6→6
k = −25→22
l = −19→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.226
S = 1.04
4326 reflections
212 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1282P)^2 + 0.4119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 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}	Occ. (<1)
C1	1.0018 (3)	0.42976 (9)	0.49998 (9)	0.0282 (4)	
H1	0.999141	0.381739	0.500818	0.034*	
C2	0.8338 (3)	0.46547 (9)	0.54090 (9)	0.0271 (4)	
C3	0.8250 (3)	0.53703 (9)	0.54249 (9)	0.0263 (4)	
C4	0.6417 (3)	0.57248 (9)	0.58429 (9)	0.0293 (4)	
H4	0.541486	0.545774	0.614439	0.035*	
C5	0.6004 (3)	0.63941 (9)	0.58438 (10)	0.0315 (4)	
H5	0.703009	0.665749	0.554545	0.038*	
C6	0.4164 (3)	0.67620 (9)	0.62495 (10)	0.0305 (4)	
C7	0.2447 (4)	0.64463 (9)	0.66949 (10)	0.0328 (4)	
H7	0.241720	0.596658	0.671825	0.039*	
C8	0.0809 (4)	0.68086 (10)	0.70980 (10)	0.0342 (4)	
H8	−0.032467	0.657429	0.739139	0.041*	
C9	0.0776 (3)	0.75238 (10)	0.70852 (10)	0.0321 (4)	
C10	0.2425 (4)	0.78409 (9)	0.66190 (11)	0.0356 (5)	
H10	0.241220	0.831968	0.657671	0.043*	
C11	0.4067 (4)	0.74642 (10)	0.62209 (11)	0.0353 (5)	
H11	0.517277	0.769477	0.591587	0.042*	
N12	−0.0778 (3)	0.78916 (8)	0.75092 (9)	0.0378 (4)	
C13	−0.2493 (4)	0.75584 (11)	0.79867 (11)	0.0384 (5)	
H13A	−0.328316	0.716066	0.773025	0.046*	
H13B	−0.390006	0.787388	0.808745	0.046*	
C14	−0.1140 (5)	0.73267 (13)	0.87110 (12)	0.0509 (6)	
H14A	−0.045434	0.772655	0.898586	0.061*	
H14B	0.033702	0.703325	0.861314	0.061*	
C15	−0.2961 (6)	0.69376 (17)	0.91778 (14)	0.0680 (8)	
H15A	−0.430100	0.725048	0.933255	0.082*	
H15B	−0.383733	0.657786	0.887739	0.082*	
C16	−0.1571 (8)	0.6619 (2)	0.98509 (17)	0.0979 (13)	
H16A	−0.280814	0.636417	1.011912	0.147*	
H16B	−0.078315	0.697489	1.016516	0.147*	
H16C	−0.022530	0.631301	0.970201	0.147*	
C17	−0.0411 (4)	0.86162 (10)	0.76109 (12)	0.0429 (5)	
H17A	0.144060	0.872210	0.758497	0.051*	
H17B	−0.088147	0.873902	0.810547	0.051*	
C18	−0.1977 (4)	0.90508 (11)	0.70557 (14)	0.0513 (6)	
H18A	−0.154804	0.892381	0.655846	0.062*	
H18B	−0.383637	0.896162	0.709179	0.062*	
C19	−0.1453 (7)	0.98008 (13)	0.7174 (2)	0.0813 (10)	
H19A	0.041342	0.988786	0.714964	0.098*	0.876 (10)
H19B	−0.191815	0.992952	0.766774	0.098*	0.876 (10)
H19C	−0.196449	0.991878	0.766620	0.098*	0.124 (10)
H19D	−0.261038	1.005300	0.681792	0.098*	0.124 (10)
C20	−0.2980 (10)	1.02394 (18)	0.6607 (3)	0.1071 (19)	0.876 (10)
H20A	−0.265212	1.008472	0.611580	0.161*	0.876 (10)

H20B	−0.243776	1.071191	0.666704	0.161*	0.876 (10)
H20C	−0.482582	1.020207	0.667333	0.161*	0.876 (10)
C20A	0.133 (8)	1.0069 (14)	0.711 (3)	0.14 (2)	0.124 (10)
H20D	0.257434	0.974759	0.734686	0.214*	0.124 (10)
H20E	0.152878	1.050830	0.735716	0.214*	0.124 (10)
H20F	0.165532	1.011855	0.659804	0.214*	0.124 (10)
C21	0.6589 (3)	0.42723 (9)	0.58235 (9)	0.0299 (4)	
N22	0.5191 (3)	0.39710 (9)	0.61504 (9)	0.0410 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0233 (8)	0.0305 (8)	0.0319 (9)	0.0016 (7)	0.0087 (7)	−0.0003 (7)
C2	0.0190 (8)	0.0348 (9)	0.0284 (9)	−0.0012 (7)	0.0083 (7)	0.0003 (7)
C3	0.0197 (8)	0.0326 (9)	0.0274 (9)	0.0007 (7)	0.0062 (7)	−0.0014 (7)
C4	0.0211 (8)	0.0372 (9)	0.0308 (9)	0.0005 (7)	0.0099 (7)	−0.0022 (7)
C5	0.0250 (9)	0.0365 (9)	0.0344 (10)	−0.0011 (7)	0.0120 (8)	−0.0039 (7)
C6	0.0242 (9)	0.0362 (9)	0.0320 (9)	0.0016 (7)	0.0084 (7)	−0.0047 (7)
C7	0.0287 (9)	0.0343 (9)	0.0369 (10)	0.0009 (7)	0.0122 (8)	−0.0043 (7)
C8	0.0268 (9)	0.0408 (10)	0.0364 (10)	−0.0003 (8)	0.0128 (8)	−0.0045 (8)
C9	0.0225 (8)	0.0398 (10)	0.0345 (10)	0.0029 (7)	0.0067 (8)	−0.0086 (8)
C10	0.0309 (10)	0.0348 (9)	0.0424 (11)	0.0016 (8)	0.0115 (8)	−0.0053 (8)
C11	0.0283 (9)	0.0384 (10)	0.0408 (11)	−0.0001 (8)	0.0142 (8)	−0.0036 (8)
N12	0.0306 (8)	0.0404 (9)	0.0444 (10)	0.0020 (7)	0.0164 (7)	−0.0118 (7)
C13	0.0283 (9)	0.0480 (11)	0.0408 (11)	0.0043 (8)	0.0145 (8)	−0.0090 (9)
C14	0.0413 (12)	0.0692 (14)	0.0433 (12)	0.0094 (11)	0.0108 (10)	−0.0102 (11)
C15	0.0702 (18)	0.090 (2)	0.0464 (14)	0.0094 (16)	0.0169 (13)	0.0042 (13)
C16	0.121 (3)	0.116 (3)	0.0606 (19)	0.045 (2)	0.027 (2)	0.0141 (18)
C17	0.0307 (10)	0.0463 (11)	0.0532 (13)	−0.0007 (9)	0.0135 (9)	−0.0185 (9)
C18	0.0397 (12)	0.0417 (11)	0.0732 (16)	0.0022 (10)	0.0079 (11)	−0.0121 (11)
C19	0.085 (2)	0.0429 (13)	0.115 (3)	0.0015 (15)	0.000 (2)	−0.0127 (15)
C20	0.129 (4)	0.0492 (19)	0.138 (4)	0.011 (2)	−0.019 (3)	0.005 (2)
C20A	0.14 (4)	0.047 (15)	0.24 (5)	0.008 (18)	0.01 (3)	−0.05 (2)
C21	0.0239 (9)	0.0364 (9)	0.0306 (9)	0.0023 (7)	0.0089 (7)	0.0014 (7)
N22	0.0337 (9)	0.0476 (9)	0.0433 (10)	−0.0017 (8)	0.0142 (8)	0.0099 (8)

Geometric parameters (Å, º)

C1—C2	1.389 (2)	C14—H14A	0.9900
C1—C3^{i}	1.400 (2)	C14—H14B	0.9900
C1—H1	0.9500	C15—C16	1.521 (4)
C2—C3	1.416 (2)	C15—H15A	0.9900
C2—C21	1.445 (2)	C15—H15B	0.9900
C3—C4	1.450 (2)	C16—H16A	0.9800
C4—C5	1.341 (3)	C16—H16B	0.9800
C4—H4	0.9500	C16—H16C	0.9800
C5—C6	1.453 (2)	C17—C18	1.522 (3)
C5—H5	0.9500	C17—H17A	0.9900

C6—C11	1.391 (3)	C17—H17B	0.9900
C6—C7	1.404 (2)	C18—C19	1.521 (3)
C7—C8	1.373 (2)	C18—H18A	0.9900
C7—H7	0.9500	C18—H18B	0.9900
C8—C9	1.415 (3)	C19—C20	1.531 (5)
C8—H8	0.9500	C19—C20A	1.55 (4)
C9—N12	1.374 (2)	C19—H19A	0.9900
C9—C10	1.406 (3)	C19—H19B	0.9900
C10—C11	1.384 (2)	C19—H19C	0.9900
C10—H10	0.9500	C19—H19D	0.9900
C11—H11	0.9500	C20—H20A	0.9800
N12—C17	1.456 (3)	C20—H20B	0.9800
N12—C13	1.457 (2)	C20—H20C	0.9800
C13—C14	1.528 (3)	C20A—H20D	0.9800
C13—H13A	0.9900	C20A—H20E	0.9800
C13—H13B	0.9900	C20A—H20F	0.9800
C14—C15	1.533 (4)	C21—N22	1.145 (2)

C2—C1—C3^{i}	121.47 (16)	C16—C15—H15A	109.0
C2—C1—H1	119.3	C14—C15—H15A	109.0
C3^{i}—C1—H1	119.3	C16—C15—H15B	109.0
C1—C2—C3	122.83 (15)	C14—C15—H15B	109.0
C1—C2—C21	117.86 (16)	H15A—C15—H15B	107.8
C3—C2—C21	119.30 (15)	C15—C16—H16A	109.5
C1^{i}—C3—C2	115.70 (14)	C15—C16—H16B	109.5
C1^{i}—C3—C4	123.10 (16)	H16A—C16—H16B	109.5
C2—C3—C4	121.18 (15)	C15—C16—H16C	109.5
C5—C4—C3	126.14 (16)	H16A—C16—H16C	109.5
C5—C4—H4	116.9	H16B—C16—H16C	109.5
C3—C4—H4	116.9	N12—C17—C18	114.31 (18)
C4—C5—C6	127.37 (16)	N12—C17—H17A	108.7
C4—C5—H5	116.3	C18—C17—H17A	108.7
C6—C5—H5	116.3	N12—C17—H17B	108.7
C11—C6—C7	116.32 (15)	C18—C17—H17B	108.7
C11—C6—C5	120.28 (16)	H17A—C17—H17B	107.6
C7—C6—C5	123.39 (16)	C19—C18—C17	111.9 (2)
C8—C7—C6	122.12 (17)	C19—C18—H18A	109.2
C8—C7—H7	118.9	C17—C18—H18A	109.2
C6—C7—H7	118.9	C19—C18—H18B	109.2
C7—C8—C9	121.33 (17)	C17—C18—H18B	109.2
C7—C8—H8	119.3	H18A—C18—H18B	107.9
C9—C8—H8	119.3	C18—C19—C20	112.1 (3)
N12—C9—C10	121.53 (17)	C18—C19—C20A	118.7 (10)
N12—C9—C8	121.80 (16)	C18—C19—H19A	109.2
C10—C9—C8	116.67 (15)	C20—C19—H19A	109.2
C11—C10—C9	120.83 (17)	C18—C19—H19B	109.2
C11—C10—H10	119.6	C20—C19—H19B	109.2
C9—C10—H10	119.6	H19A—C19—H19B	107.9

C10—C11—C6	122.65 (17)	C18—C19—H19C	107.6
C10—C11—H11	118.7	C20A—C19—H19C	107.6
C6—C11—H11	118.7	C18—C19—H19D	107.6
C9—N12—C17	121.14 (16)	C20A—C19—H19D	107.6
C9—N12—C13	121.12 (16)	H19C—C19—H19D	107.1
C17—N12—C13	116.63 (15)	C19—C20—H20A	109.5
N12—C13—C14	113.52 (17)	C19—C20—H20B	109.5
N12—C13—H13A	108.9	H20A—C20—H20B	109.5
C14—C13—H13A	108.9	C19—C20—H20C	109.5
N12—C13—H13B	108.9	H20A—C20—H20C	109.5
C14—C13—H13B	108.9	H20B—C20—H20C	109.5
H13A—C13—H13B	107.7	C19—C20A—H20D	109.5
C13—C14—C15	112.1 (2)	C19—C20A—H20E	109.5
C13—C14—H14A	109.2	H20D—C20A—H20E	109.5
C15—C14—H14A	109.2	C19—C20A—H20F	109.5
C13—C14—H14B	109.2	H20D—C20A—H20F	109.5
C15—C14—H14B	109.2	H20E—C20A—H20F	109.5
H14A—C14—H14B	107.9	N22—C21—C2	179.6 (2)
C16—C15—C14	112.8 (3)		

C3^{i}—C1—C2—C3	0.2 (3)	C8—C9—C10—C11	−2.7 (3)
C3^{i}—C1—C2—C21	179.14 (16)	C9—C10—C11—C6	0.8 (3)
C1—C2—C3—C1^{i}	−0.2 (3)	C7—C6—C11—C10	1.5 (3)
C21—C2—C3—C1^{i}	−179.11 (16)	C5—C6—C11—C10	−177.36 (18)
C1—C2—C3—C4	178.23 (16)	C10—C9—N12—C17	−12.9 (3)
C21—C2—C3—C4	−0.7 (3)	C8—C9—N12—C17	166.80 (19)
C1^{i}—C3—C4—C5	4.8 (3)	C10—C9—N12—C13	179.57 (18)
C2—C3—C4—C5	−173.47 (19)	C8—C9—N12—C13	−0.8 (3)
C3—C4—C5—C6	179.23 (17)	C9—N12—C13—C14	81.1 (2)
C4—C5—C6—C11	176.5 (2)	C17—N12—C13—C14	−87.0 (2)
C4—C5—C6—C7	−2.2 (3)	N12—C13—C14—C15	−176.24 (19)
C11—C6—C7—C8	−1.8 (3)	C13—C14—C15—C16	172.0 (2)
C5—C6—C7—C8	176.99 (18)	C9—N12—C17—C18	91.0 (2)
C6—C7—C8—C9	−0.1 (3)	C13—N12—C17—C18	−100.9 (2)
C7—C8—C9—N12	−177.27 (18)	N12—C17—C18—C19	−178.2 (2)
C7—C8—C9—C10	2.4 (3)	C17—C18—C19—C20	178.7 (3)
N12—C9—C10—C11	176.95 (18)	C17—C18—C19—C20A	61 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13*B*···N22^{ii}	0.99	2.70	3.555 (3)	145

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