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3-(2,4-Difluoroanilino)-9-nitrodibenzo-[*b*,*e*]oxepin-11(6*H*)-one

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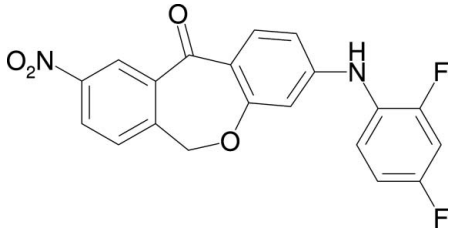
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.127; data-to-parameter ratio = 11.9.

In the title compound, $C_{20}H_{12}F_2N_2O_4$, the two benzene rings of the tricyclic unit are oriented at a dihedral angle of 30.6 (1)°. The 2,4-difluoroanilino residue is oriented at a dihedral angle of 68.2 (1)° with respect to the phenoxy ring. In the crystal, N—H···O hydrogen bonds between the amino group and the carbonyl O atom of the oxepinone ring link the molecules into infinte chains along the c axis.

Related literature

For palladium-catalysed amination reactions of aryl halides with anilines, see: Jensen *et al.* (2004). For p38 MAP kinase inhibitors based on dibenzo[*b*,*e*]oxepin-11(6*H*)-one, see: Laufer *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{12}F_2N_2O_4$ M_r = 382.32
Orthorhombic, $Pna2_1$
a = 27.0813 (15) Å
b = 13.0411 (8) Å
c = 4.5998 (2) Å
V = 1624.51 (15) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 193 K
0.47 × 0.24 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: numerical (*CORINC*; Dräger & Gattow, 1971)
T_{min} = 0.721, T_{max} = 0.882
3417 measured reflections
3010 independent reflections
2924 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
3 standard reflections every 60 min
intensity decay: 3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.127
S = 1.03
3010 reflections
253 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack, (1983), 1270 Friedel pairs
Flack parameter: −0.22 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
N16—H16···O25^{i}	0.95	2.32	3.236 (3)	162

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CORINC* (Dräger & Gattow, 1971); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2261).

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supporting information

Acta Cryst. (2011). E**67**, o555 [doi:10.1107/S1600536811002881]

3-(2,4-Difluoroanilino)-9-nitrodibenzo[*b*,*e*]oxepin-11(6*H*)-one

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S1. Comment

Based on dibenzo[b,e]oxepin-11(6*H*)-one (Laufer *et al.* 2006) as p38 MAP kinase inhibitors, our intent was to synthesize disubstituted oxepin derivatives. The title compound was synthesized in the course of an ongoing study to increase the solubility of the molecules. The structure of the title compound, at 193 K shows orthorhombic symmetry. The two phenyl rings of the tricyclic unit are oriented at a dihedral angle of 30.6 (1°). The 2,4-difluoroanilino residue is oriented at a dihedral angel of 68.2 (1°) towards the phenoxy ring. The crystal stucture is characterized by an intermolecular hydrogen bond N16–H···O25 (2.32 Å).

S2. Experimental

For the preperation of the title compound a mixture of 200 mg (0.69 mmol) 3-chloro-9-nitrodibenzo[b,e]oxepin-11(6*H*)-one, 100 mg (0.77 mmol) 2–4-difluoroaniline, 1.00 g (3.07 mmol) Cs_2CO_3, 45 mg (0.10 mmol) 2-(dicyclohexyl-phosphino)-2`-4`-6`-triisopropylbiphenyl and 20 mg (0.09 mmol) $Pd(OAc)_2$ in 2 ml absolute *tert*-butanol and 10 ml absolute 2.4-dioxane was stirred for 1 h at 284 K under an argon atmosphere. The mixture was then filtered and evaporated under reduced pressure. The residue was purified by flash chromatography (SiO_2 n-hexane/ethyl acetate 2:1) to get 103 mg (0,27 mmol) of the product as a yellow solid (yield 39 %). Crystals of the title compound were obtained by slow evaporation of diethyl ether and hexane (1:1) at room temperature.

S3. Refinement

Hydrogen atoms attached to carbons were placed at calculated positions with C—H = 0.95 Å (aromatic) or 0.98–0.99 Å (sp^3 C-atom). Hydrogen atom attached to nitrogen was located in diff. Fourier maps. All H atoms were refined in the riding-model approximation with isotropic displacement parameters (set at 1.2–1.5 times of the U_{eq} of the parent atom). The absolute structure was determined on the basis of 1270 Friedel pairs.

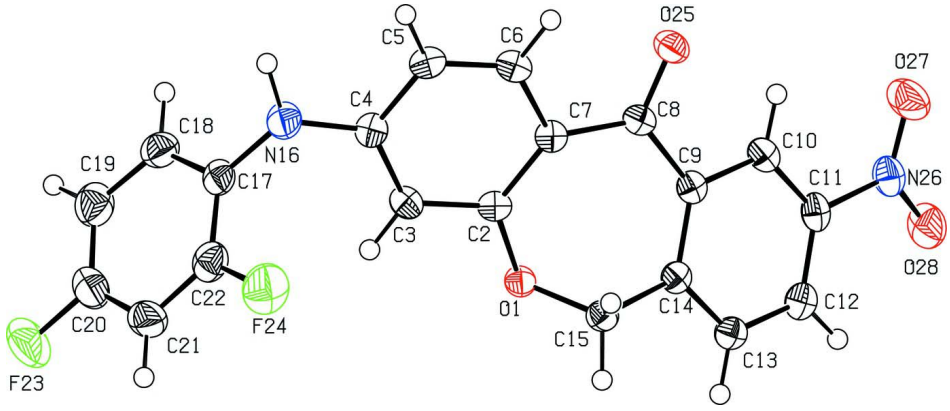

Figure 1

View of compound **I**. Displacement ellipsoids are drawn at the 50% probability level.

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$V = 1624.51\ (15)$ Å^3
$Z = 4$
$F(000) = 784$
$D_x = 1.563$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 65$–$69°$
$\mu = 1.08$ mm^{-1}
$T = 193$ K
Needle, yellow
0.47 × 0.24 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: rotating anode
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: numerical (CORINC; Dräger & Gattow, 1971)
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3010 independent reflections
2924 reflections with $I > 2\sigma(I)$
$R_{int} = 0.051$
$\theta_{max} = 69.8°$, $\theta_{min} = 3.3°$
$h = -33\rightarrow33$
$k = -15\rightarrow15$
$l = -5\rightarrow5$
3 standard reflections every 60 min
intensity decay: 3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.127$
$S = 1.03$
3010 reflections
253 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0989P)^2 + 0.3414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.023$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Absolute structure: Flack, (1983), 1270 Friedel pairs
Absolute structure parameter: −0.22 (18)

Special details

Experimental. ^{1}H NMR (200 MHz, DMSO-d~6~) δ in p.p.m. 5.32 (s, 2 H), 6.26 (m, 1 H), 6.65 (dd, *J*=8.65, 1.96 Hz, 1 H), 7.11 (m, 1 H), 7.39 (m, 2 H), 7.82 (m, 1 H), 8.02 (d, *J*=8.97 Hz, 1 H), 8.41 (dd, *J*=8.21, 2.53 Hz, 1 H), 8.52 (d, *J*=2.40 Hz, 1 H), 8.85 (s, NH,1 H).
^{13}C NMR (50 MHz, DMSO-d~6~) δ in p.p.m. 72.5, 102.1, 110.5, 116.5, 124.3, 127.0, 130.4, 134.1, 141.1, 142.9, 148.3, 152.9, 163.4, 185.1, C—F not detected.
GC/MS, *m/z* (%) 382 (100, M^+), 308 (12), 152 (9), 98 (7), 63 (1).

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.58864 (5)	0.24963 (11)	0.3890 (3)	0.0240 (3)
C2	0.56177 (7)	0.30020 (15)	0.5965 (4)	0.0215 (4)
C3	0.51656 (8)	0.25513 (16)	0.6587 (5)	0.0242 (4)
H3	0.5068	0.1947	0.5587	0.029*
C4	0.48548 (8)	0.29789 (17)	0.8665 (5)	0.0245 (4)
C5	0.50161 (8)	0.38484 (16)	1.0212 (5)	0.0242 (4)
H5	0.4818	0.4123	1.1728	0.029*
C6	0.54556 (8)	0.42947 (15)	0.9536 (5)	0.0234 (4)
H6	0.5556	0.4882	1.0605	0.028*
C7	0.57698 (7)	0.39218 (15)	0.7306 (4)	0.0216 (4)
C8	0.61655 (7)	0.46277 (15)	0.6377 (4)	0.0222 (4)
C9	0.65513 (7)	0.43587 (15)	0.4150 (5)	0.0215 (4)
C10	0.68194 (8)	0.51865 (17)	0.3032 (5)	0.0248 (4)
H10	0.6752	0.5865	0.3670	0.030*
C11	0.71823 (7)	0.50081 (16)	0.0997 (5)	0.0262 (5)
C12	0.73012 (8)	0.40368 (18)	0.0000 (5)	0.0275 (5)
H12	0.7551	0.3936	−0.1423	0.033*
C13	0.70420 (7)	0.32175 (17)	0.1161 (5)	0.0253 (5)
H13	0.7120	0.2541	0.0550	0.030*
C14	0.66696 (7)	0.33663 (16)	0.3204 (5)	0.0223 (4)
C15	0.64067 (7)	0.24498 (15)	0.4420 (5)	0.0253 (5)
H15A	0.6542	0.1820	0.3525	0.030*
H15B	0.6466	0.2412	0.6541	0.030*
N16	0.43947 (7)	0.25975 (16)	0.9317 (5)	0.0341 (5)
H16	0.4191	0.3040	1.0435	0.041*
C17	0.41597 (8)	0.18098 (18)	0.7713 (5)	0.0287 (5)
C18	0.37502 (8)	0.20134 (19)	0.5998 (6)	0.0352 (5)
H18	0.3631	0.2697	0.5860	0.042*
C19	0.35112 (10)	0.1240 (2)	0.4481 (7)	0.0434 (6)
H19	0.3226	0.1381	0.3345	0.052*

C20	0.36991 (10)	0.0266 (2)	0.4670 (6)	0.0407 (6)
C21	0.41046 (10)	0.00166 (19)	0.6308 (7)	0.0409 (6)
H21	0.4229	−0.0664	0.6384	0.049*
C22	0.43238 (9)	0.0805 (2)	0.7842 (6)	0.0355 (6)
F23	0.34769 (7)	−0.04940 (15)	0.3148 (5)	0.0629 (6)
F24	0.47133 (6)	0.05902 (13)	0.9539 (5)	0.0558 (5)
O25	0.61751 (6)	0.55042 (11)	0.7364 (4)	0.0302 (4)
N26	0.74461 (7)	0.58919 (15)	−0.0221 (5)	0.0315 (4)
O27	0.73855 (7)	0.67347 (14)	0.0898 (5)	0.0476 (5)
O28	0.77170 (7)	0.57374 (15)	−0.2321 (5)	0.0434 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0251 (7)	0.0263 (7)	0.0205 (8)	−0.0019 (5)	0.0021 (6)	−0.0047 (6)
C2	0.0275 (9)	0.0227 (10)	0.0143 (9)	0.0030 (7)	−0.0011 (8)	0.0020 (8)
C3	0.0306 (10)	0.0249 (10)	0.0171 (10)	−0.0024 (8)	−0.0015 (9)	−0.0011 (8)
C4	0.0270 (10)	0.0287 (10)	0.0179 (11)	−0.0006 (8)	0.0009 (8)	0.0029 (8)
C5	0.0303 (10)	0.0286 (11)	0.0137 (10)	0.0044 (8)	0.0011 (8)	0.0012 (8)
C6	0.0327 (10)	0.0243 (9)	0.0132 (10)	0.0013 (8)	−0.0043 (8)	0.0005 (8)
C7	0.0253 (9)	0.0251 (10)	0.0142 (10)	0.0013 (8)	−0.0036 (8)	0.0021 (8)
C8	0.0271 (9)	0.0210 (9)	0.0184 (10)	0.0019 (7)	−0.0060 (8)	0.0015 (8)
C9	0.0230 (9)	0.0245 (9)	0.0170 (10)	−0.0001 (8)	−0.0063 (8)	0.0033 (8)
C10	0.0283 (10)	0.0227 (9)	0.0234 (11)	−0.0015 (8)	−0.0083 (9)	0.0037 (8)
C11	0.0246 (9)	0.0300 (11)	0.0239 (11)	−0.0059 (8)	−0.0052 (8)	0.0067 (9)
C12	0.0252 (9)	0.0333 (11)	0.0239 (11)	−0.0003 (8)	−0.0023 (9)	0.0038 (9)
C13	0.0256 (9)	0.0261 (10)	0.0241 (11)	0.0017 (8)	−0.0032 (9)	0.0014 (8)
C14	0.0218 (9)	0.0249 (10)	0.0201 (10)	0.0013 (7)	−0.0055 (8)	0.0019 (8)
C15	0.0266 (10)	0.0220 (10)	0.0275 (11)	0.0005 (7)	0.0022 (9)	0.0028 (9)
N16	0.0318 (9)	0.0404 (11)	0.0301 (11)	−0.0050 (8)	0.0088 (9)	−0.0101 (9)
C17	0.0274 (10)	0.0336 (11)	0.0250 (12)	−0.0039 (8)	0.0078 (9)	−0.0015 (9)
C18	0.0338 (11)	0.0355 (13)	0.0363 (14)	0.0036 (9)	0.0046 (10)	−0.0016 (11)
C19	0.0371 (12)	0.0532 (15)	0.0400 (16)	−0.0028 (11)	−0.0025 (12)	−0.0075 (13)
C20	0.0447 (14)	0.0424 (13)	0.0349 (15)	−0.0147 (11)	0.0132 (11)	−0.0110 (11)
C21	0.0444 (12)	0.0287 (12)	0.0495 (16)	−0.0035 (10)	0.0142 (12)	0.0015 (12)
C22	0.0309 (11)	0.0381 (12)	0.0373 (14)	−0.0009 (9)	0.0052 (11)	0.0077 (11)
F23	0.0677 (11)	0.0604 (11)	0.0606 (12)	−0.0257 (9)	0.0120 (10)	−0.0305 (10)
F24	0.0483 (9)	0.0541 (10)	0.0649 (12)	0.0051 (7)	−0.0134 (9)	0.0171 (9)
O25	0.0352 (8)	0.0244 (8)	0.0311 (9)	−0.0034 (6)	0.0017 (7)	−0.0047 (7)
N26	0.0312 (9)	0.0318 (10)	0.0314 (11)	−0.0070 (8)	−0.0010 (9)	0.0060 (9)
O27	0.0584 (11)	0.0300 (9)	0.0545 (13)	−0.0103 (8)	0.0147 (10)	0.0022 (8)
O28	0.0460 (9)	0.0441 (10)	0.0402 (11)	−0.0120 (8)	0.0137 (9)	0.0031 (9)

Geometric parameters (Å, º)

O1—C2	1.370 (2)	C12—H12	0.9500
O1—C15	1.431 (3)	C13—C14	1.392 (3)
C2—C3	1.388 (3)	C13—H13	0.9500

C2—C7	1.410 (3)	C14—C15	1.499 (3)
C3—C4	1.390 (3)	C15—H15A	0.9900
C3—H3	0.9500	C15—H15B	0.9900
C4—N16	1.375 (3)	N16—C17	1.416 (3)
C4—C5	1.408 (3)	N16—H16	0.9504
C5—C6	1.361 (3)	C17—C18	1.387 (3)
C5—H5	0.9500	C17—C22	1.385 (3)
C6—C7	1.419 (3)	C18—C19	1.387 (4)
C6—H6	0.9500	C18—H18	0.9500
C7—C8	1.476 (3)	C19—C20	1.371 (4)
C8—O25	1.230 (3)	C19—H19	0.9500
C8—C9	1.504 (3)	C20—F23	1.355 (3)
C9—C10	1.399 (3)	C20—C21	1.371 (4)
C9—C14	1.403 (3)	C21—C22	1.381 (4)
C10—C11	1.377 (3)	C21—H21	0.9500
C10—H10	0.9500	C22—F24	1.341 (3)
C11—C12	1.385 (3)	N26—O27	1.225 (3)
C11—N26	1.467 (3)	N26—O28	1.230 (3)
C12—C13	1.385 (3)		

C2—O1—C15	115.13 (16)	C12—C13—H13	119.3
O1—C2—C3	114.11 (19)	C14—C13—H13	119.3
O1—C2—C7	123.99 (18)	C13—C14—C9	120.24 (19)
C3—C2—C7	121.85 (19)	C13—C14—C15	119.00 (19)
C2—C3—C4	120.4 (2)	C9—C14—C15	120.75 (19)
C2—C3—H3	119.8	O1—C15—C14	111.72 (16)
C4—C3—H3	119.8	O1—C15—H15A	109.3
N16—C4—C3	123.6 (2)	C14—C15—H15A	109.3
N16—C4—C5	117.53 (19)	O1—C15—H15B	109.3
C3—C4—C5	118.85 (19)	C14—C15—H15B	109.3
C6—C5—C4	120.02 (19)	H15A—C15—H15B	107.9
C6—C5—H5	120.0	C4—N16—C17	123.8 (2)
C4—C5—H5	120.0	C4—N16—H16	115.2
C5—C6—C7	122.89 (19)	C17—N16—H16	117.5
C5—C6—H6	118.6	C18—C17—C22	117.5 (2)
C7—C6—H6	118.6	C18—C17—N16	121.1 (2)
C2—C7—C6	115.63 (18)	C22—C17—N16	121.3 (2)
C2—C7—C8	128.01 (18)	C17—C18—C19	121.4 (2)
C6—C7—C8	115.54 (18)	C17—C18—H18	119.3
O25—C8—C7	119.20 (19)	C19—C18—H18	119.3
O25—C8—C9	116.95 (18)	C20—C19—C18	117.9 (2)
C7—C8—C9	123.78 (18)	C20—C19—H19	121.0
C10—C9—C14	118.6 (2)	C18—C19—H19	121.0
C10—C9—C8	115.52 (18)	F23—C20—C19	118.7 (3)
C14—C9—C8	125.81 (18)	F23—C20—C21	117.8 (3)
C11—C10—C9	119.3 (2)	C19—C20—C21	123.5 (2)
C11—C10—H10	120.3	C20—C21—C22	116.6 (2)
C9—C10—H10	120.3	C20—C21—H21	121.7

C10—C11—C12	123.1 (2)	C22—C21—H21	121.7
C10—C11—N26	118.3 (2)	F24—C22—C21	118.7 (2)
C12—C11—N26	118.6 (2)	F24—C22—C17	118.3 (2)
C11—C12—C13	117.4 (2)	C21—C22—C17	123.0 (2)
C11—C12—H12	121.3	O27—N26—O28	123.8 (2)
C13—C12—H12	121.3	O27—N26—C11	118.7 (2)
C12—C13—C14	121.3 (2)	O28—N26—C11	117.5 (2)

C15—O1—C2—C3	−140.97 (18)	C12—C13—C14—C9	−0.5 (3)
C15—O1—C2—C7	41.3 (3)	C12—C13—C14—C15	−179.1 (2)
O1—C2—C3—C4	179.62 (18)	C10—C9—C14—C13	−0.9 (3)
C7—C2—C3—C4	−2.6 (3)	C8—C9—C14—C13	−178.83 (19)
C2—C3—C4—N16	177.5 (2)	C10—C9—C14—C15	177.64 (19)
C2—C3—C4—C5	−2.8 (3)	C8—C9—C14—C15	−0.3 (3)
N16—C4—C5—C6	−176.1 (2)	C2—O1—C15—C14	−88.1 (2)
C3—C4—C5—C6	4.2 (3)	C13—C14—C15—O1	−121.5 (2)
C4—C5—C6—C7	−0.2 (3)	C9—C14—C15—O1	59.9 (3)
O1—C2—C7—C6	−176.19 (18)	C3—C4—N16—C17	−8.2 (4)
C3—C2—C7—C6	6.3 (3)	C5—C4—N16—C17	172.1 (2)
O1—C2—C7—C8	14.7 (3)	C4—N16—C17—C18	−110.1 (3)
C3—C2—C7—C8	−162.8 (2)	C4—N16—C17—C22	71.2 (3)
C5—C6—C7—C2	−4.9 (3)	C22—C17—C18—C19	0.4 (4)
C5—C6—C7—C8	165.57 (19)	N16—C17—C18—C19	−178.4 (2)
C2—C7—C8—O25	162.9 (2)	C17—C18—C19—C20	−1.5 (4)
C6—C7—C8—O25	−6.2 (3)	C18—C19—C20—F23	−178.5 (2)
C2—C7—C8—C9	−14.0 (3)	C18—C19—C20—C21	1.0 (4)
C6—C7—C8—C9	176.95 (17)	F23—C20—C21—C22	−179.9 (2)
O25—C8—C9—C10	−11.8 (3)	C19—C20—C21—C22	0.6 (4)
C7—C8—C9—C10	165.16 (18)	C20—C21—C22—F24	178.1 (2)
O25—C8—C9—C14	166.2 (2)	C20—C21—C22—C17	−1.8 (4)
C7—C8—C9—C14	−16.9 (3)	C18—C17—C22—F24	−178.6 (2)
C14—C9—C10—C11	1.4 (3)	N16—C17—C22—F24	0.1 (3)
C8—C9—C10—C11	179.54 (17)	C18—C17—C22—C21	1.3 (4)
C9—C10—C11—C12	−0.6 (3)	N16—C17—C22—C21	−179.9 (2)
C9—C10—C11—N26	177.82 (18)	C10—C11—N26—O27	10.3 (3)
C10—C11—C12—C13	−0.8 (3)	C12—C11—N26—O27	−171.3 (2)
N26—C11—C12—C13	−179.2 (2)	C10—C11—N26—O28	−169.8 (2)
C11—C12—C13—C14	1.3 (3)	C12—C11—N26—O28	8.7 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N16—H16···O25^{i}	0.95	2.32	3.236 (3)	162

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