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N,N'-{[Bis(trifluoromethyl)methylene]di-*p*-phenylene}diphthalimide

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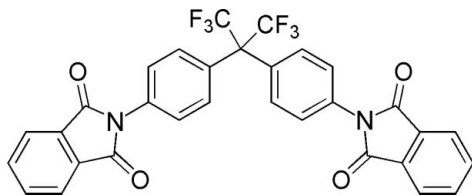
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Key indicators: single-crystal X-ray study; $T = 292$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.066; wR factor = 0.169; data-to-parameter ratio = 11.2.

The molecule of the title compound, $\text{C}_{31}\text{H}_{16}\text{F}_6\text{N}_2\text{O}_4$, consists of two phthalimide units linked by a [bis(trifluoromethyl)methylene]di-*p*-phenylene bridge, with the two halves of the molecule related to each other by a twofold rotation axis. The dihedral angle between the planes of the two central benzene rings is $70.5(3)^\circ$. The terminal isoindole groups are approximately planar, with a maximum r.m.s. deviation of 0.006 Å from the mean plane, and they form dihedral angles of $46.03(3)^\circ$ to the attached benzene rings. Intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link neighboring molecules into chains along the c axis.

Related literature

For details of the biological activity and uses of bis(imide) derivatives, see: Rich *et al.* (1975); Degenhardt *et al.* (2002); Mallakpour & Kowsari (2004); Zhang *et al.* (1999); Langhals & Kirner (2000); Yakimov & Forrest (2002). For a related structure, see: Li *et al.* (2007).



Experimental

Crystal data

$\text{C}_{31}\text{H}_{16}\text{F}_6\text{N}_2\text{O}_4$
 $M_r = 594.46$
Orthorhombic, *Pcca*
 $a = 13.3588(19)$ Å
 $b = 12.5340(18)$ Å
 $c = 15.792(2)$ Å
 $V = 2644.2(6)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.13$ mm⁻¹
 $T = 292(2)$ K
 $0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
15610 measured reflections
2607 independent reflections
1864 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.119$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$
 $wR(F^2) = 0.168$
 $S = 1.05$
2607 reflections
232 parameters
64 restraints
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.23$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C15}-\text{H15}\cdots\text{O1}^i$	0.93	2.42	3.199 (4)	141

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: EZZ112).

References

- Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART* (Version 5.054) and *SAINTE* (Version 6.01). Bruker AXS Inc., Madison, Wisconsin, USA.
Degenhardt, C. F., Smith, M. D. & Shimizu, K. D. (2002). *Org. Lett.* **4**, 723–726.
Langhals, H. & Kirner, S. (2000). *Eur. J. Org. Chem.* pp. 365–380.
Li, J., Li, Y.-T. & Wang, Z.-H. (2007). *Acta Cryst.* **E63**, o3420.
Mallakpour, S. & Kowsari, E. (2004). *J. Appl. Polym. Sci.* **91**, 2992–3000.
Rich, D. H., Gesellchen, P. D., Tong, A., Cheung, A. & Buckner, C. K. (1975). *J. Med. Chem.* **18**, 1004–1010.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Yakimov, A. & Forrest, S. R. (2002). *Appl. Phys. Lett.* **81**, 3085–3087.
Zhang, Q., Hamilton, D. G., Feeder, N., Teat, S. J., Goodman, J. M. & Sanders, J. K. (1999). *New J. Chem.* **23**, 897–903.

supplementary materials

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N,N'-{[Bis(trifluoromethyl)methylene]di-*p*-phenylene}diphthalimide

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Comment

Bisimides are heterocyclic compounds that sometimes exhibit biological activity (Rich *et al.*, 1975). Moreover, they are synthetic precursors with applications in organic synthesis (Degenhardt *et al.*, 2002), polymer synthesis (Mallakpour & Kowsari, 2004), supramolecular chemistry (Zhang *et al.*, 1999), and for the development of new materials (Langhals & Kirner, 2000) and molecular electronic devices (Yakimov & Forrest, 2002).

Following our studies on the synthesis of bisimides derivatives (Li *et al.*, 2007), we report here the structure of the title compound (I), Fig. 1. In the molecule, two phthalimide units are linked by a (1,1-di-trifluoromethyl)-methylenedi-*p*-phenylene bridge. The dihedral angle between the planes of the two central benzene rings is 70.5 (3)°. The terminal isoindole group is approximately planar with a maximum r.m.s. deviation of 0.006 Å from the best fit plane by C11 and makes a dihedral angle of 46.03 (3)° to the attached central benzene ring. Intermolecular C—H···O hydrogen bonds contribute to the stability of the structure (Table 1).

Experimental

A solution of phthaloyl dichloride (420 mg, 2 mmol) was added slowly over a period of 10 min to a solution of 4-(2-(4-aminophenyl)-1,1,1,3,3,3-hexafluoropropan-2-yl)benzenamine (334 mg, 1 mmol) in dichloromethane (25 ml) at 273 K to yield a light yellow precipitate. Triethylamine (5 ml) was then added to dissolve the precipitate which became a yellow suspension after stirring for 12 h. The compound was filtered and dried to give (I), (yield 362 mg, 61%). Single crystals of (I) were obtained by recrystallization from DMF at room temperature.

Refinement

Non-hydrogen atoms were refined with anisotropic displacement parameters. One of the trifluoromethyl groups (C1/F1/F2/F3) of the title compound was found to be disordered over two orientations. The occupancies of the disordered positions C1/C1', F1/F1', F2/F2' and F3/F3' were refined to 0.59 (5)/0.41 (5). All H atoms were initially located in a difference Fourier map and then included with constrained bond lengths and isotropic displacement parameters: C—H=0.93 Å and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{C})$ for aromatic H atoms.

Figures

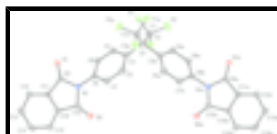


Fig. 1. The molecular structure of (I) showing atom labels with 50% probability displacement ellipsoids.

N,N'-[Bis(trifluoromethyl)methylene]di-*p*-phenylene}diphthalimide

Crystal data

$C_{31}H_{16}F_6N_2O_4$	$F_{000} = 1208$
$M_r = 594.46$	$D_x = 1.493 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pcca</i>	Mo $K\alpha$ radiation
Hall symbol: -P 2a 2ac	$\lambda = 0.71073 \text{ \AA}$
$a = 13.3588 (19) \text{ \AA}$	Cell parameters from 2679 reflections
$b = 12.5340 (18) \text{ \AA}$	$\theta = 2.6\text{--}21.8^\circ$
$c = 15.792 (2) \text{ \AA}$	$\mu = 0.13 \text{ mm}^{-1}$
$V = 2644.2 (6) \text{ \AA}^3$	$T = 292 (2) \text{ K}$
$Z = 4$	Block, colorless
	$0.30 \times 0.30 \times 0.20 \text{ mm}$

Data collection

Bruker SMART 4K CCD area-detector diffractometer	1864 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.119$
Monochromator: graphite	$\theta_{\text{max}} = 26.0^\circ$
$T = 292(2) \text{ K}$	$\theta_{\text{min}} = 2.6^\circ$
φ and ω scans	$h = -16 \rightarrow 16$
Absorption correction: none	$k = -15 \rightarrow 13$
15610 measured reflections	$l = -19 \rightarrow 19$
2607 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.168$	$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2 + 1.4164P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
2607 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
232 parameters	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
64 restraints	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.1413 (6)	0.5169 (6)	0.0925 (5)	0.061 (3)	0.59
F1	0.1409 (5)	0.5845 (3)	0.0233 (3)	0.110 (2)	0.59
F2	0.0992 (5)	0.4244 (3)	0.0577 (3)	0.115 (2)	0.59
F3	0.0585 (4)	0.5547 (4)	0.1406 (4)	0.0905 (18)	0.59
C1'	0.1891 (7)	0.5093 (6)	0.0641 (4)	0.067 (3)	0.41
F1'	0.2253 (6)	0.5779 (5)	0.0078 (4)	0.088 (2)	0.41
F2'	0.1774 (6)	0.4132 (4)	0.0295 (4)	0.083 (2)	0.41
F3'	0.1045 (5)	0.5408 (7)	0.1022 (6)	0.072 (3)	0.41
C2	0.2500	0.5000	0.1377 (3)	0.089 (2)	
C3	0.2705 (3)	0.6000 (2)	0.1916 (2)	0.0590 (10)	
C4	0.2369 (3)	0.7005 (3)	0.1690 (2)	0.0572 (10)	
H4	0.1967	0.7089	0.1214	0.069*	
C5	0.3309 (3)	0.5905 (3)	0.2625 (2)	0.0641 (11)	
H5	0.3531	0.5233	0.2788	0.077*	
C6	0.2630 (3)	0.7884 (2)	0.21707 (19)	0.0460 (8)	
H6	0.2388	0.8554	0.2022	0.055*	
C7	0.3592 (3)	0.6783 (3)	0.3097 (2)	0.0555 (9)	
H7	0.4011	0.6706	0.3564	0.067*	
C8	0.3240 (2)	0.7780 (2)	0.28632 (19)	0.0419 (7)	
C9	0.3798 (2)	0.9679 (2)	0.29929 (19)	0.0414 (7)	
C10	0.3466 (2)	0.8763 (3)	0.42443 (19)	0.0414 (7)	
C11	0.3948 (2)	1.0421 (2)	0.37121 (19)	0.0404 (7)	
C12	0.4248 (3)	1.1469 (3)	0.3716 (2)	0.0517 (9)	
H12	0.4403	1.1826	0.3217	0.062*	
C13	0.4310 (3)	1.1972 (3)	0.4497 (2)	0.0595 (10)	
H13	0.4506	1.2683	0.4522	0.071*	
C14	0.4084 (3)	1.1434 (3)	0.5240 (2)	0.0560 (10)	
H14	0.4129	1.1791	0.5755	0.067*	
C15	0.3795 (2)	1.0383 (3)	0.5228 (2)	0.0500 (9)	
H15	0.3648	1.0021	0.5726	0.060*	
C16	0.3731 (2)	0.9880 (2)	0.44536 (18)	0.0382 (7)	
N1	0.35108 (19)	0.86997 (19)	0.33529 (15)	0.0405 (6)	
O1	0.38753 (18)	0.98510 (18)	0.22441 (13)	0.0569 (7)	
O3	0.32502 (19)	0.80458 (19)	0.47064 (14)	0.0570 (7)	

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.104 (8)	0.039 (5)	0.040 (4)	0.000 (5)	-0.012 (5)	0.007 (4)
F1	0.228 (7)	0.043 (2)	0.060 (3)	-0.030 (4)	-0.054 (4)	0.018 (2)
F2	0.200 (6)	0.041 (2)	0.105 (4)	-0.026 (3)	-0.081 (5)	0.001 (2)
F3	0.091 (4)	0.067 (3)	0.114 (5)	-0.007 (3)	-0.036 (3)	0.013 (3)
C1'	0.129 (8)	0.038 (5)	0.033 (5)	-0.027 (6)	0.005 (5)	-0.008 (4)
F1'	0.146 (6)	0.055 (4)	0.061 (4)	-0.008 (5)	-0.025 (5)	0.007 (3)
F2'	0.120 (5)	0.053 (4)	0.075 (5)	-0.010 (4)	-0.040 (4)	-0.014 (3)
F3'	0.046 (5)	0.055 (5)	0.115 (8)	0.016 (4)	-0.029 (4)	-0.005 (5)
C2	0.199 (8)	0.028 (3)	0.039 (3)	-0.018 (4)	0.000	0.000
C3	0.107 (3)	0.0301 (17)	0.0400 (19)	-0.0091 (18)	0.004 (2)	0.0000 (14)
C4	0.095 (3)	0.0373 (18)	0.0391 (18)	-0.0116 (18)	-0.0078 (19)	0.0001 (14)
C5	0.111 (3)	0.0280 (17)	0.053 (2)	0.0087 (18)	-0.003 (2)	0.0038 (15)
C6	0.071 (2)	0.0292 (15)	0.0377 (17)	-0.0012 (15)	-0.0008 (16)	0.0028 (13)
C7	0.076 (2)	0.0424 (19)	0.048 (2)	0.0042 (17)	-0.0049 (18)	0.0026 (16)
C8	0.0587 (19)	0.0338 (16)	0.0333 (16)	-0.0039 (14)	0.0052 (15)	-0.0013 (13)
C9	0.0523 (19)	0.0385 (17)	0.0333 (17)	-0.0040 (14)	0.0012 (14)	0.0000 (13)
C10	0.0429 (17)	0.0455 (19)	0.0358 (17)	0.0020 (14)	0.0023 (13)	0.0026 (15)
C11	0.0427 (16)	0.0434 (18)	0.0351 (17)	-0.0030 (13)	0.0015 (14)	-0.0020 (13)
C12	0.063 (2)	0.0432 (19)	0.049 (2)	-0.0073 (16)	0.0010 (17)	-0.0029 (16)
C13	0.062 (2)	0.049 (2)	0.068 (3)	-0.0036 (17)	-0.0006 (19)	-0.0192 (19)
C14	0.0503 (19)	0.068 (3)	0.049 (2)	0.0047 (17)	-0.0017 (16)	-0.0275 (18)
C15	0.0458 (18)	0.068 (2)	0.0362 (18)	0.0035 (16)	-0.0020 (15)	-0.0117 (16)
C16	0.0369 (16)	0.0454 (18)	0.0322 (15)	0.0037 (13)	-0.0015 (13)	-0.0020 (13)
N1	0.0558 (15)	0.0345 (14)	0.0313 (14)	-0.0033 (12)	-0.0005 (12)	-0.0015 (11)
O1	0.0885 (18)	0.0518 (14)	0.0305 (12)	-0.0178 (12)	0.0006 (12)	0.0018 (10)
O3	0.0754 (16)	0.0545 (15)	0.0411 (13)	-0.0073 (12)	0.0015 (12)	0.0129 (11)

Geometric parameters (\AA , $^\circ$)

C1—F1	1.382 (7)	C5—H5	0.9300
C1—F2	1.401 (8)	C6—C8	1.370 (4)
C1—F3	1.422 (8)	C6—H6	0.9300
C1—C2	1.632 (7)	C7—C8	1.386 (4)
C1'—F1'	1.329 (8)	C7—H7	0.9300
C1'—F2'	1.332 (7)	C8—N1	1.434 (4)
C1'—F3'	1.339 (8)	C9—O1	1.207 (4)
C1'—C2	1.423 (7)	C9—N1	1.406 (4)
C1'—C1 ⁱ	1.645 (18)	C9—C11	1.482 (4)
C1'—F1 ⁱ	1.815 (12)	C10—O3	1.194 (4)
F1'—F2 ⁱ	1.350 (11)	C10—N1	1.411 (4)
F1'—C1 ⁱ	1.815 (12)	C10—C16	1.481 (4)
F2'—F1 ⁱ	1.350 (11)	C11—C12	1.373 (4)
C2—C1 ⁱ	1.423 (7)	C11—C16	1.383 (4)

C2—C3	1.540 (4)	C12—C13	1.387 (5)
C2—C3 ⁱ	1.540 (4)	C12—H12	0.9300
C2—C1 ⁱ	1.632 (7)	C13—C14	1.386 (5)
C3—C4	1.384 (5)	C13—H13	0.9300
C3—C5	1.386 (5)	C14—C15	1.374 (5)
C4—C6	1.383 (4)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.378 (4)
C5—C7	1.381 (5)	C15—H15	0.9300
F1—C1—F2	101.3 (5)	C6—C4—C3	120.1 (3)
F1—C1—F3	102.4 (6)	C6—C4—H4	119.9
F2—C1—F3	100.0 (6)	C3—C4—H4	119.9
F1—C1—C2	115.3 (6)	C7—C5—C3	121.8 (3)
F2—C1—C2	114.9 (5)	C7—C5—H5	119.1
F3—C1—C2	120.1 (6)	C3—C5—H5	119.1
F1'—C1'—F2'	110.6 (6)	C8—C6—C4	120.8 (3)
F1'—C1'—F3'	114.7 (8)	C8—C6—H6	119.6
F2'—C1'—F3'	110.6 (7)	C4—C6—H6	119.6
F1'—C1'—C2	113.0 (6)	C5—C7—C8	118.8 (3)
F2'—C1'—C2	109.2 (7)	C5—C7—H7	120.6
F3'—C1'—C2	98.1 (6)	C8—C7—H7	120.6
F1'—C1'—C1 ⁱⁱ	74.4 (6)	C6—C8—C7	120.0 (3)
F2'—C1'—C1 ⁱⁱ	89.3 (7)	C6—C8—N1	120.3 (3)
F3'—C1'—C1 ⁱⁱ	151.2 (6)	C7—C8—N1	119.7 (3)
C2—C1'—C1 ⁱⁱ	54.7 (4)	O1—C9—N1	125.2 (3)
F1'—C1'—F1 ⁱⁱ	80.3 (6)	O1—C9—C11	128.9 (3)
F2'—C1'—F1 ⁱⁱ	47.8 (5)	N1—C9—C11	105.9 (2)
F3'—C1'—F1 ⁱⁱ	158.3 (7)	O3—C10—N1	125.3 (3)
C2—C1'—F1 ⁱⁱ	89.4 (6)	O3—C10—C16	129.3 (3)
C1 ⁱⁱ —C1'—F1 ⁱⁱ	44.8 (4)	N1—C10—C16	105.4 (3)
C1'—F1'—F2 ⁱⁱ	103.5 (6)	C12—C11—C16	121.7 (3)
C1'—F1'—C1 ⁱⁱ	60.8 (6)	C12—C11—C9	130.1 (3)
F2 ⁱⁱ —F1'—C1 ⁱⁱ	47.0 (4)	C16—C11—C9	108.2 (3)
C1'—F2'—F1 ⁱⁱ	85.2 (6)	C11—C12—C13	117.2 (3)
C1'—C2—C1 ⁱⁱ	70.6 (8)	C11—C12—H12	121.4
C1'—C2—C3	119.1 (3)	C13—C12—H12	121.4
C1 ⁱⁱ —C2—C3	114.6 (4)	C14—C13—C12	121.2 (3)
C1'—C2—C3 ⁱ	114.6 (4)	C14—C13—H13	119.4
C1 ⁱⁱ —C2—C3 ⁱ	119.1 (3)	C12—C13—H13	119.4
C3—C2—C3 ⁱ	112.9 (4)	C15—C14—C13	121.1 (3)
C1'—C2—C1 ⁱ	99.4 (6)	C15—C14—H14	119.5
C1 ⁱⁱ —C2—C1 ⁱ	28.8 (4)	C13—C14—H14	119.5
C3—C2—C1 ⁱ	100.9 (3)	C14—C15—C16	117.9 (3)
C3 ⁱ —C2—C1 ⁱ	107.1 (3)	C14—C15—H15	121.0
C1'—C2—C1	28.8 (4)	C16—C15—H15	121.0

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C1 ⁱ —C2—C1	99.4 (6)	C15—C16—C11	120.9 (3)
C3—C2—C1	107.1 (3)	C15—C16—C10	130.1 (3)
C3 ⁱ —C2—C1	100.9 (3)	C11—C16—C10	108.9 (3)
C1 ⁱ —C2—C1	128.2 (7)	C9—N1—C10	111.5 (2)
C4—C3—C5	118.4 (3)	C9—N1—C8	123.5 (2)
C4—C3—C2	122.7 (3)	C10—N1—C8	124.9 (2)
C5—C3—C2	118.8 (3)		
F2'—C1'—F1'—F2 ⁱ	-103.3 (7)	C1'—C2—C3—C4	-3.8 (6)
F3'—C1'—F1'—F2 ⁱ	130.7 (8)	C1 ⁱ —C2—C3—C4	76.8 (6)
C2—C1'—F1'—F2 ⁱ	19.4 (8)	C3 ⁱ —C2—C3—C4	-142.5 (4)
C1 ⁱ —C1'—F1'—F2 ⁱ	-20.2 (6)	C1 ⁱ —C2—C3—C4	103.5 (5)
F1 ⁱ —C1'—F1'—F2 ⁱ	-65.8 (7)	C1—C2—C3—C4	-32.4 (5)
F2'—C1'—F1'—C1 ⁱ	-83.2 (8)	C1'—C2—C3—C5	-179.2 (5)
F3'—C1'—F1'—C1 ⁱ	150.9 (8)	C1 ⁱ —C2—C3—C5	-98.6 (6)
C2—C1'—F1'—C1 ⁱ	39.6 (5)	C3 ⁱ —C2—C3—C5	42.1 (3)
F1 ⁱ —C1'—F1'—C1 ⁱ	-45.6 (4)	C1 ⁱ —C2—C3—C5	-71.9 (5)
F1'—C1'—F2'—F1 ⁱ	54.2 (8)	C1—C2—C3—C5	152.2 (4)
F3'—C1'—F2'—F1 ⁱ	-177.6 (8)	C5—C3—C4—C6	-0.5 (6)
C2—C1'—F2'—F1 ⁱ	-70.8 (7)	C2—C3—C4—C6	-175.9 (3)
C1 ⁱ —C1'—F2'—F1 ⁱ	-18.8 (5)	C4—C3—C5—C7	-1.0 (6)
F1'—C1'—C2—C1 ⁱ	-48.7 (5)	C2—C3—C5—C7	174.6 (3)
F2'—C1'—C2—C1 ⁱ	74.8 (7)	C3—C4—C6—C8	1.5 (5)
F3'—C1'—C2—C1 ⁱ	-170.0 (9)	C3—C5—C7—C8	1.5 (6)
F1 ⁱ —C1'—C2—C1 ⁱ	30.4 (3)	C4—C6—C8—C7	-0.9 (5)
F1'—C1'—C2—C3	59.2 (8)	C4—C6—C8—N1	179.5 (3)
F2'—C1'—C2—C3	-177.2 (5)	C5—C7—C8—C6	-0.5 (5)
F3'—C1'—C2—C3	-62.0 (7)	C5—C7—C8—N1	179.0 (3)
C1 ⁱ —C1'—C2—C3	108.0 (5)	O1—C9—C11—C12	-3.0 (6)
F1 ⁱ —C1'—C2—C3	138.4 (4)	N1—C9—C11—C12	178.6 (3)
F1'—C1'—C2—C3 ⁱ	-162.7 (5)	O1—C9—C11—C16	177.2 (3)
F2'—C1'—C2—C3 ⁱ	-39.1 (8)	N1—C9—C11—C16	-1.2 (3)
F3'—C1'—C2—C3 ⁱ	76.1 (7)	C16—C11—C12—C13	-1.0 (5)
C1 ⁱ —C1'—C2—C3 ⁱ	-114.0 (5)	C9—C11—C12—C13	179.2 (3)
F1 ⁱ —C1'—C2—C3 ⁱ	-83.5 (5)	C11—C12—C13—C14	0.5 (5)
F1'—C1'—C2—C1 ⁱ	-48.9 (7)	C12—C13—C14—C15	0.2 (5)
F2'—C1'—C2—C1 ⁱ	74.7 (7)	C13—C14—C15—C16	-0.4 (5)
F3'—C1'—C2—C1 ⁱ	-170.1 (6)	C14—C15—C16—C11	-0.2 (5)
C1 ⁱ —C1'—C2—C1 ⁱ	-0.2 (6)	C14—C15—C16—C10	178.5 (3)
F1 ⁱ —C1'—C2—C1 ⁱ	30.3 (5)	C12—C11—C16—C15	0.9 (5)
F1'—C1'—C2—C1	130.9 (12)	C9—C11—C16—C15	-179.2 (3)
F2'—C1'—C2—C1	-105.5 (12)	C12—C11—C16—C10	-178.0 (3)
F3'—C1'—C2—C1	9.7 (8)	C9—C11—C16—C10	1.8 (3)

C1 ⁱ —C1'—C2—C1	179.7 (12)	O3—C10—C16—C15	-0.3 (6)
F1 ⁱ —C1'—C2—C1	-149.9 (11)	N1—C10—C16—C15	179.4 (3)
F1—C1—C2—C1'	-42.3 (8)	O3—C10—C16—C11	178.6 (3)
F2—C1—C2—C1'	75.0 (10)	N1—C10—C16—C11	-1.7 (3)
F3—C1—C2—C1'	-165.7 (13)	O1—C9—N1—C10	-178.4 (3)
F1—C1—C2—C1 ⁱ	-42.0 (7)	C11—C9—N1—C10	0.0 (3)
F2—C1—C2—C1 ⁱ	75.3 (7)	O1—C9—N1—C8	-2.0 (5)
F3—C1—C2—C1 ⁱ	-165.4 (6)	C11—C9—N1—C8	176.4 (3)
F1—C1—C2—C3	77.5 (7)	O3—C10—N1—C9	-179.3 (3)
F2—C1—C2—C3	-165.2 (5)	C16—C10—N1—C9	1.0 (3)
F3—C1—C2—C3	-45.9 (7)	O3—C10—N1—C8	4.4 (5)
F1—C1—C2—C3 ⁱ	-164.3 (5)	C16—C10—N1—C8	-175.3 (3)
F2—C1—C2—C3 ⁱ	-47.0 (7)	C6—C8—N1—C9	-43.6 (4)
F3—C1—C2—C3 ⁱ	72.4 (6)	C7—C8—N1—C9	136.9 (3)
F1—C1—C2—C1 ⁱ	-42.1 (5)	C6—C8—N1—C10	132.3 (3)
F2—C1—C2—C1 ⁱ	75.2 (6)	C7—C8—N1—C10	-47.2 (4)
F3—C1—C2—C1 ⁱ	-165.5 (7)		

Symmetry codes: (i) $-x+1/2, -y+1, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C15—H15 \cdots O1 ⁱⁱ	0.93	2.42	3.199 (4)	141

Symmetry codes: (ii) $x, -y+2, z+1/2$.

Fig. 1

