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1-(4-Methoxyphenyl)-2-[4-(trifluoromethyl)phenyl]-1*H*-phenanthro[9,10-*d*]imidazole

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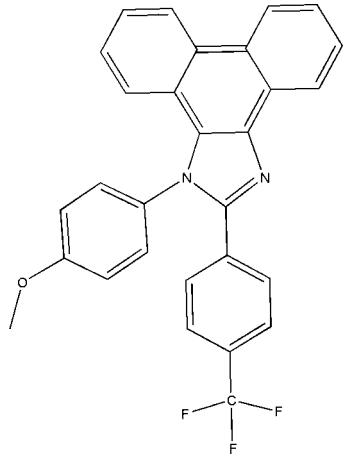
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.045; wR factor = 0.124; data-to-parameter ratio = 16.2.

In the title compound, $C_{29}H_{19}F_3N_2O$, a phenanthroline-fused imidazole tetracyclic system, the fused benzene rings deviate slightly from the central ring and make dihedral angles with this ring of 3.47 (8) and 3.05 (8)°. The trifluoromethylphenyl ring is roughly coplanar with the phenanthroline-fused imidazole tetracyclic system [dihedral angle = 11.02 (6)°], while the methoxyphenyl ring is almost perpendicular [dihedral angle = 87.65 (6)°]. There are intramolecular C—H $\cdots\pi$ interactions involving the methoxyphenyl ring and the central phenanthroline ring, as well as an intermolecular C—H$\cdots\pi$ interaction involving the phenanthroline ring. In addition, there is an intermolecular π–π interaction involving the central phenanthroline ring and the trifluoromethylphenyl ring [centroid–centroid distance = 3.685 (2) Å], as well as C—H$\cdots$N interactions linking the molecules into dimers.

Related literature

For background to the supramolecular architecture of phenanthroline compounds, see: Lehn (1995). For metal sensors, see: Walters *et al.* (2000). For molecular electronics, see: Peng *et al.* (1997). For photo sensitizers see: Hara *et al.* (2001). For a related structure, see: Sathishkumar *et al.* (2013).



Experimental

Crystal data

$C_{29}H_{19}F_3N_2O$
M_r = 468.46
Monoclinic, $P2_1/c$
a = 11.7063 (9) Å
b = 20.2301 (16) Å
c = 9.5419 (8) Å
β = 99.725 (2)°
V = 2227.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.32 × 0.29 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.956, T_{max} = 0.999
24449 measured reflections
5128 independent reflections
3511 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.124
S = 1.01
5128 reflections
317 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 and *Cg* are the centroids of the methoxyphenyl and phenthroline rings, repsectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C28—H28$\cdots$N2^{i}	0.95	2.55	3.402 (2)	150
C3—H3$\cdots$*Cg*1	0.95	2.86	3.719 (2)	154
C10—H10$\cdots$*Cg*2^{ii}	0.95	2.69	3.419 (2)	136
C17—H17$\cdots$*Cg*1	0.95	2.74	3.6042 (2)	154

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2* and *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

The authors thank Dr Babu Varghese, Senior Scientific Officer SAIF, IIT Chennai, India, for carrying out the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2223).

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1-(4-Methoxyphenyl)-2-[4-(trifluoromethyl)phenyl]-1*H*-phenanthro[9,10-*d*]imidazole

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S1. Comment

The large variety of complexes based on phenanthroline or polypyridyl derivatives allows the formation of many different molecular systems with various applications ranging from metallo-supramolecular chemistry (Lehn, 1995), metal sensors (Walters *et al.*, 2000), molecular electronics (Peng *et al.*, 1997), and photo sensitizers (Hara *et al.*, 2001). Therefore, in the recent years the preparation of phenanthroimidazoles has gained great attention.

In this phenanthroline triclinic ring system, the phenyl rings on either end are slightly deviated from the central ring and make the dihedral angles with this ring of 3.47 (8)° and 3.05 (8)° respectively. The trifluromethyl phenyl ring is almost coplanar with the phenanthroline fused imidazole tetracyclic system (dihedral angle of 11.02 (6)°) while methoxy phenyl ring is almost perpendicular (dihedral angle of 87.65 (6)°).

The maximum deviation of C9 atom from the mean plane of the tetracyclic phenantherene fused imidazole ring is 0.078 (2)° and that of C29 atom from the methoxy phenyl ring is -0.043 (3)°. The C22 atom of the trifluromethyl phenyl ring is deviated by -0.040 (2)°.

There are intramolecular C3—H3 ···π and C17—H17···π (methoxyphenyl ring system) interactions as well as an intermolecular C10—H10···π interaction involving the phenanthroline ring (at the symmetry code *x*, 1/2 - y, 1/2 + *z*). There is an intermolecular π–π interaction involving the central ring phenanthroline ring and the trifluoromethyl phenyl ring (Cg···Cg 3.685 Å, 1-x, -y, 2-*z*). In addition there C—H···N out-of-plane interactions linking the molecules into dimers as shown in Fig. 2.

S2. Experimental

A mixture of phenanthrene-9,10-dione (1.0 g,4.8 mmol), ammonium acetate (1.48 g,19.2 mmol), 4-trifluromethyl-benzaldehyde(0.83 g,4.8 mmol) and 4-methoxyaniline (2.95 g,24 mmol) have been refluxed in ethanol (20 mL) at 80°C. The reaction was monitored by TLC and purified by column chromatography using petroleum ether:ethyl acetate (9:1) as the eluent.Yield: 0.74 g (51%)

S3. Refinement

All the hydrogen atoms were geometrically fixed and allowed to ride on their parent atoms with C—H= 0.93 - 0.97 Å,and U_{iso}(H) = 1.3U_{eq}(C)

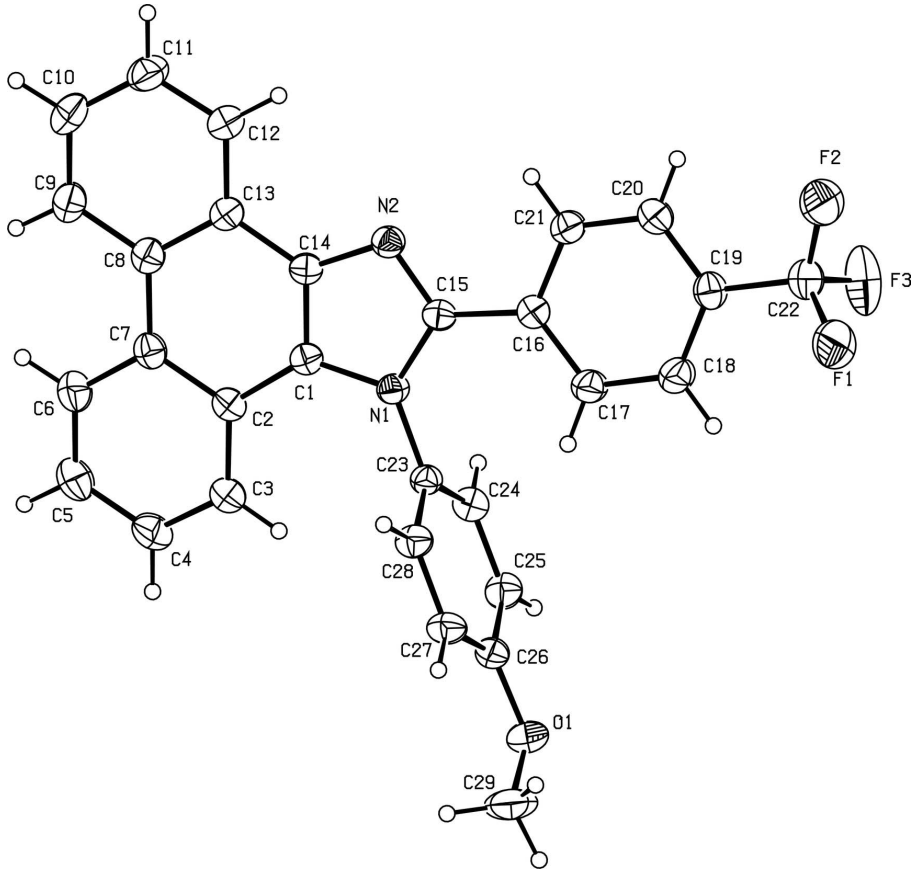

Figure 1

The molecular structure and labelling scheme for (I) with displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

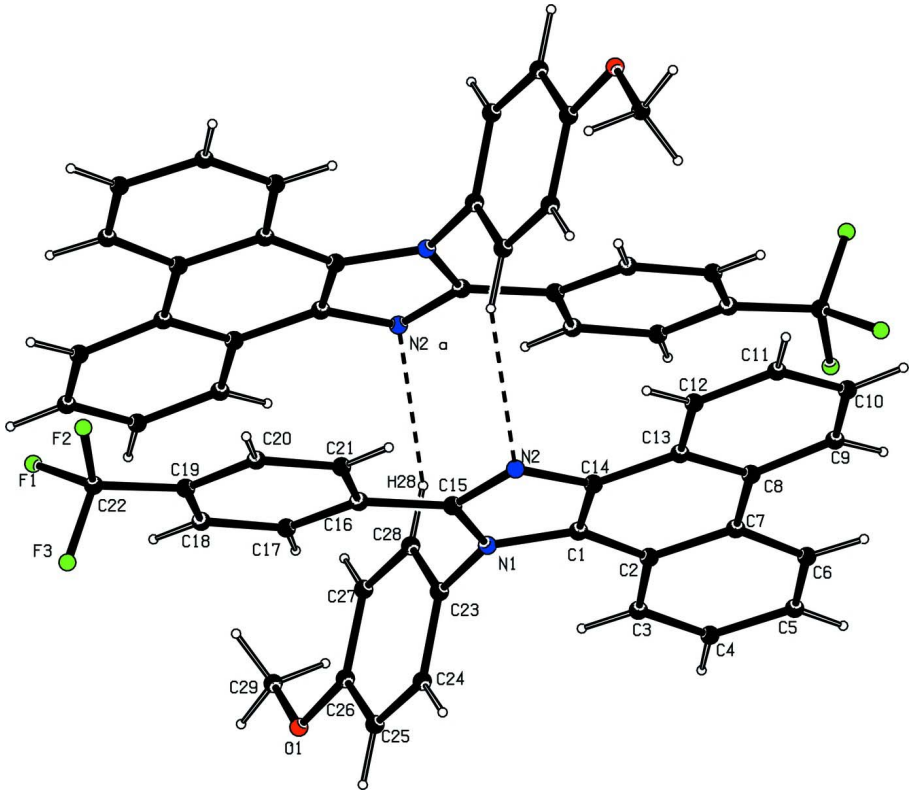

Figure 2

A diagram showing the C-H···N out of plane π interactions linking molecules into dimers.A packing diagram for (I) is shown.

1-(4-Methoxyphenyl)-2-[4-(trifluromethyl)phenyl]-1*H*-phenanthro[9,10-*d*]imidazole

Crystal data

$C_{29}H_{19}F_3N_2O$
$M_r = 468.46$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.7063\ (9)$ Å
$b = 20.2301\ (16)$ Å
$c = 9.5419\ (8)$ Å
$\beta = 99.725\ (2)°$
$V = 2227.2\ (3)$ Å^3
$Z = 4$
$F(000) = 968$
$D_x = 1.397$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5131 reflections
$\theta = 1.8–27.6°$
$\mu = 0.10$ mm^{-1}
$T = 173$ K
Block, colourless
0.32 × 0.29 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.956$, $T_{max} = 0.999$
24449 measured reflections
5128 independent reflections
3511 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 27.6°$, $\theta_{min} = 2.4°$
$h = -15\rightarrow14$
$k = 0\rightarrow26$
$l = 0\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.124$
$S = 1.01$
5128 reflections
317 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.6328P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.94082 (11)	−0.18352 (6)	0.83630 (17)	0.0945 (5)
F2	1.03787 (11)	−0.09609 (7)	0.88946 (19)	0.1026 (5)
F3	0.97313 (14)	−0.11886 (9)	0.67561 (17)	0.1112 (6)
O1	0.24682 (11)	−0.21387 (6)	0.47694 (14)	0.0615 (4)
N1	0.41440 (11)	0.01373 (6)	0.76779 (13)	0.0381 (3)
N2	0.53956 (11)	0.08671 (6)	0.88301 (14)	0.0414 (3)
C1	0.34962 (13)	0.06745 (7)	0.80056 (16)	0.0375 (3)
C2	0.22709 (13)	0.08118 (8)	0.77095 (16)	0.0404 (4)
C3	0.14290 (15)	0.04019 (9)	0.69130 (19)	0.0516 (4)
H3	0.1656	−0.0009	0.6565	0.062*
C4	0.02892 (16)	0.05872 (11)	0.6633 (2)	0.0625 (5)
H4	−0.0268	0.0306	0.6092	0.075*
C5	−0.00549 (16)	0.11848 (11)	0.7138 (2)	0.0674 (6)
H5	−0.0846	0.1313	0.6938	0.081*
C6	0.07410 (16)	0.15882 (10)	0.7921 (2)	0.0591 (5)
H6	0.0489	0.1995	0.8260	0.071*
C7	0.19225 (14)	0.14223 (8)	0.82452 (17)	0.0439 (4)
C8	0.27615 (14)	0.18711 (8)	0.90664 (17)	0.0435 (4)
C9	0.24350 (17)	0.24581 (9)	0.96904 (19)	0.0546 (4)
H9	0.1637	0.2571	0.9580	0.066*
C10	0.32367 (19)	0.28690 (9)	1.0449 (2)	0.0626 (5)
H10	0.2989	0.3260	1.0861	0.075*
C11	0.44104 (19)	0.27210 (9)	1.0624 (2)	0.0621 (5)
H11	0.4964	0.3011	1.1146	0.075*
C12	0.47650 (16)	0.21546 (8)	1.00403 (18)	0.0519 (4)

H12	0.5568	0.2053	1.0155	0.062*
C13	0.39540 (14)	0.17238 (7)	0.92748 (16)	0.0410 (4)
C14	0.42898 (13)	0.11102 (7)	0.87125 (16)	0.0387 (3)
C15	0.52887 (13)	0.02806 (7)	0.82138 (16)	0.0380 (3)
C16	0.63143 (13)	−0.01355 (7)	0.81555 (16)	0.0388 (3)
C17	0.62932 (15)	−0.07882 (8)	0.76912 (19)	0.0505 (4)
H17	0.5571	−0.1000	0.7379	0.061*
C18	0.73102 (16)	−0.11314 (9)	0.7679 (2)	0.0543 (4)
H18	0.7280	−0.1577	0.7360	0.065*
C19	0.83675 (14)	−0.08351 (8)	0.81246 (18)	0.0467 (4)
C20	0.84057 (15)	−0.01934 (9)	0.8612 (2)	0.0533 (4)
H20	0.9131	0.0013	0.8938	0.064*
C21	0.73894 (15)	0.01501 (8)	0.86267 (19)	0.0494 (4)
H21	0.7426	0.0592	0.8967	0.059*
C22	0.94602 (17)	−0.11998 (10)	0.8042 (2)	0.0606 (5)
C23	0.36937 (13)	−0.04529 (7)	0.69415 (16)	0.0374 (3)
C24	0.36221 (14)	−0.04960 (8)	0.54819 (17)	0.0434 (4)
H24	0.3855	−0.0135	0.4960	0.052*
C25	0.32095 (15)	−0.10681 (8)	0.47918 (18)	0.0482 (4)
H25	0.3165	−0.1102	0.3791	0.058*
C26	0.28607 (13)	−0.15923 (8)	0.55452 (18)	0.0450 (4)
C27	0.29213 (15)	−0.15426 (8)	0.70017 (19)	0.0502 (4)
H27	0.2676	−0.1901	0.7523	0.060*
C28	0.33403 (15)	−0.09708 (8)	0.76958 (18)	0.0460 (4)
H28	0.3384	−0.0936	0.8696	0.055*
C29	0.2023 (2)	−0.26684 (12)	0.5502 (3)	0.0963 (9)
H29A	0.1761	−0.3025	0.4830	0.144*
H29B	0.1369	−0.2510	0.5929	0.144*
H29C	0.2633	−0.2834	0.6251	0.144*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0725 (8)	0.0575 (8)	0.1538 (14)	0.0215 (6)	0.0206 (9)	0.0119 (8)
F2	0.0504 (7)	0.0934 (10)	0.1529 (14)	0.0193 (7)	−0.0148 (8)	−0.0329 (9)
F3	0.0985 (11)	0.1497 (14)	0.0970 (11)	0.0515 (10)	0.0497 (9)	0.0126 (10)
O1	0.0598 (8)	0.0564 (8)	0.0657 (8)	−0.0134 (6)	0.0028 (6)	−0.0200 (6)
N1	0.0384 (7)	0.0357 (6)	0.0391 (7)	−0.0013 (5)	0.0033 (5)	−0.0015 (5)
N2	0.0398 (7)	0.0414 (7)	0.0417 (7)	−0.0010 (6)	0.0033 (6)	−0.0023 (6)
C1	0.0414 (8)	0.0365 (8)	0.0347 (8)	−0.0008 (6)	0.0067 (6)	0.0039 (6)
C2	0.0397 (8)	0.0431 (8)	0.0383 (8)	−0.0010 (7)	0.0062 (6)	0.0059 (7)
C3	0.0422 (9)	0.0547 (10)	0.0570 (11)	−0.0020 (8)	0.0058 (8)	−0.0037 (8)
C4	0.0418 (10)	0.0735 (13)	0.0690 (13)	−0.0058 (9)	0.0002 (9)	−0.0066 (10)
C5	0.0391 (10)	0.0775 (14)	0.0831 (15)	0.0087 (10)	0.0035 (9)	0.0001 (12)
C6	0.0470 (10)	0.0600 (11)	0.0709 (13)	0.0087 (9)	0.0118 (9)	−0.0003 (10)
C7	0.0431 (9)	0.0467 (9)	0.0432 (9)	0.0031 (7)	0.0112 (7)	0.0065 (7)
C8	0.0504 (9)	0.0427 (8)	0.0392 (8)	0.0019 (7)	0.0127 (7)	0.0045 (7)
C9	0.0592 (11)	0.0505 (10)	0.0568 (11)	0.0083 (9)	0.0175 (9)	−0.0018 (8)

C10	0.0811 (14)	0.0501 (10)	0.0589 (12)	0.0058 (10)	0.0186 (10)	−0.0136 (9)
C11	0.0718 (13)	0.0532 (11)	0.0610 (12)	−0.0081 (10)	0.0102 (10)	−0.0159 (9)
C12	0.0549 (10)	0.0471 (9)	0.0536 (10)	−0.0038 (8)	0.0083 (8)	−0.0082 (8)
C13	0.0482 (9)	0.0392 (8)	0.0363 (8)	−0.0009 (7)	0.0086 (7)	0.0016 (6)
C14	0.0402 (8)	0.0379 (8)	0.0375 (8)	−0.0014 (7)	0.0054 (6)	0.0020 (6)
C15	0.0391 (8)	0.0395 (8)	0.0344 (8)	−0.0031 (7)	0.0033 (6)	0.0014 (6)
C16	0.0412 (8)	0.0412 (8)	0.0339 (8)	0.0003 (7)	0.0059 (6)	0.0029 (6)
C17	0.0427 (9)	0.0438 (9)	0.0625 (11)	−0.0007 (7)	0.0018 (8)	−0.0029 (8)
C18	0.0524 (10)	0.0424 (9)	0.0665 (12)	0.0042 (8)	0.0053 (9)	−0.0037 (8)
C19	0.0447 (9)	0.0482 (9)	0.0470 (9)	0.0067 (8)	0.0073 (7)	0.0049 (7)
C20	0.0404 (9)	0.0550 (10)	0.0629 (11)	0.0003 (8)	0.0040 (8)	−0.0046 (9)
C21	0.0458 (9)	0.0446 (9)	0.0562 (10)	−0.0001 (8)	0.0041 (8)	−0.0088 (8)
C22	0.0517 (11)	0.0564 (11)	0.0738 (14)	0.0082 (9)	0.0105 (10)	−0.0025 (10)
C23	0.0356 (8)	0.0366 (8)	0.0385 (8)	−0.0016 (6)	0.0023 (6)	−0.0017 (6)
C24	0.0452 (9)	0.0450 (9)	0.0388 (9)	−0.0016 (7)	0.0043 (7)	0.0057 (7)
C25	0.0504 (10)	0.0563 (10)	0.0355 (9)	0.0002 (8)	0.0003 (7)	−0.0043 (7)
C26	0.0357 (8)	0.0465 (9)	0.0503 (10)	−0.0025 (7)	0.0002 (7)	−0.0086 (7)
C27	0.0546 (10)	0.0447 (9)	0.0513 (10)	−0.0127 (8)	0.0091 (8)	0.0011 (8)
C28	0.0541 (10)	0.0470 (9)	0.0370 (8)	−0.0083 (8)	0.0081 (7)	−0.0012 (7)
C29	0.108 (2)	0.0749 (15)	0.112 (2)	−0.0536 (15)	0.0387 (16)	−0.0358 (14)

Geometric parameters (Å, º)

F1—C22	1.325 (2)	C11—H11	0.9500
F2—C22	1.325 (2)	C12—C13	1.400 (2)
F3—C22	1.319 (2)	C12—H12	0.9500
O1—C26	1.3661 (19)	C13—C14	1.433 (2)
O1—C29	1.425 (3)	C15—C16	1.475 (2)
N1—C15	1.3819 (19)	C16—C21	1.389 (2)
N1—C1	1.3907 (19)	C16—C17	1.392 (2)
N1—C23	1.4395 (19)	C17—C18	1.380 (2)
N2—C15	1.3209 (19)	C17—H17	0.9500
N2—C14	1.371 (2)	C18—C19	1.376 (2)
C1—C14	1.372 (2)	C18—H18	0.9500
C1—C2	1.441 (2)	C19—C20	1.377 (2)
C2—C3	1.408 (2)	C19—C22	1.490 (2)
C2—C7	1.423 (2)	C20—C21	1.380 (2)
C3—C4	1.368 (2)	C20—H20	0.9500
C3—H3	0.9500	C21—H21	0.9500
C4—C5	1.386 (3)	C23—C28	1.374 (2)
C4—H4	0.9500	C23—C24	1.384 (2)
C5—C6	1.363 (3)	C24—C25	1.378 (2)
C5—H5	0.9500	C24—H24	0.9500
C6—C7	1.406 (2)	C25—C26	1.381 (2)
C6—H6	0.9500	C25—H25	0.9500
C7—C8	1.464 (2)	C26—C27	1.383 (2)
C8—C13	1.408 (2)	C27—C28	1.381 (2)
C8—C9	1.410 (2)	C27—H27	0.9500

C9—C10	1.366 (3)	C28—H28	0.9500
C9—H9	0.9500	C29—H29A	0.9800
C10—C11	1.388 (3)	C29—H29B	0.9800
C10—H10	0.9500	C29—H29C	0.9800
C11—C12	1.369 (2)		

C26—O1—C29	117.39 (15)	N1—C15—C16	127.66 (13)
C15—N1—C1	106.52 (12)	C21—C16—C17	117.66 (15)
C15—N1—C23	127.36 (12)	C21—C16—C15	116.69 (14)
C1—N1—C23	126.12 (13)	C17—C16—C15	125.64 (14)
C15—N2—C14	105.58 (13)	C18—C17—C16	120.74 (16)
C14—C1—N1	105.24 (13)	C18—C17—H17	119.6
C14—C1—C2	122.77 (14)	C16—C17—H17	119.6
N1—C1—C2	131.98 (14)	C19—C18—C17	120.69 (16)
C3—C2—C7	119.22 (15)	C19—C18—H18	119.7
C3—C2—C1	125.09 (15)	C17—C18—H18	119.7
C7—C2—C1	115.66 (14)	C18—C19—C20	119.41 (16)
C4—C3—C2	120.96 (17)	C18—C19—C22	120.21 (16)
C4—C3—H3	119.5	C20—C19—C22	120.36 (16)
C2—C3—H3	119.5	C19—C20—C21	119.95 (16)
C3—C4—C5	120.16 (18)	C19—C20—H20	120.0
C3—C4—H4	119.9	C21—C20—H20	120.0
C5—C4—H4	119.9	C20—C21—C16	121.52 (16)
C6—C5—C4	120.07 (18)	C20—C21—H21	119.2
C6—C5—H5	120.0	C16—C21—H21	119.2
C4—C5—H5	120.0	F3—C22—F2	105.49 (18)
C5—C6—C7	122.25 (18)	F3—C22—F1	105.03 (17)
C5—C6—H6	118.9	F2—C22—F1	106.03 (17)
C7—C6—H6	118.9	F3—C22—C19	112.60 (17)
C6—C7—C2	117.35 (16)	F2—C22—C19	113.69 (17)
C6—C7—C8	121.05 (16)	F1—C22—C19	113.25 (16)
C2—C7—C8	121.58 (14)	C28—C23—C24	120.45 (14)
C13—C8—C9	116.85 (16)	C28—C23—N1	119.65 (13)
C13—C8—C7	120.25 (14)	C24—C23—N1	119.91 (13)
C9—C8—C7	122.90 (16)	C25—C24—C23	119.38 (15)
C10—C9—C8	121.69 (18)	C25—C24—H24	120.3
C10—C9—H9	119.2	C23—C24—H24	120.3
C8—C9—H9	119.2	C24—C25—C26	120.45 (15)
C9—C10—C11	120.66 (17)	C24—C25—H25	119.8
C9—C10—H10	119.7	C26—C25—H25	119.8
C11—C10—H10	119.7	O1—C26—C25	116.18 (15)
C12—C11—C10	119.56 (18)	O1—C26—C27	123.97 (16)
C12—C11—H11	120.2	C25—C26—C27	119.85 (15)
C10—C11—H11	120.2	C28—C27—C26	119.76 (15)
C11—C12—C13	120.53 (18)	C28—C27—H27	120.1
C11—C12—H12	119.7	C26—C27—H27	120.1
C13—C12—H12	119.7	C23—C28—C27	120.10 (15)
C12—C13—C8	120.70 (15)	C23—C28—H28	120.0

C12—C13—C14	121.98 (15)	C27—C28—H28	120.0
C8—C13—C14	117.29 (14)	O1—C29—H29A	109.5
N2—C14—C1	111.17 (13)	O1—C29—H29B	109.5
N2—C14—C13	126.49 (14)	H29A—C29—H29B	109.5
C1—C14—C13	122.31 (14)	O1—C29—H29C	109.5
N2—C15—N1	111.48 (13)	H29A—C29—H29C	109.5
N2—C15—C16	120.86 (13)	H29B—C29—H29C	109.5

C15—N1—C1—C14	0.30 (16)	C8—C13—C14—C1	−0.5 (2)
C23—N1—C1—C14	179.48 (13)	C14—N2—C15—N1	0.87 (17)
C15—N1—C1—C2	179.13 (15)	C14—N2—C15—C16	−179.16 (13)
C23—N1—C1—C2	−1.7 (2)	C1—N1—C15—N2	−0.75 (16)
C14—C1—C2—C3	175.80 (16)	C23—N1—C15—N2	−179.92 (13)
N1—C1—C2—C3	−2.9 (3)	C1—N1—C15—C16	179.28 (14)
C14—C1—C2—C7	−2.3 (2)	C23—N1—C15—C16	0.1 (2)
N1—C1—C2—C7	179.08 (15)	N2—C15—C16—C21	−7.2 (2)
C7—C2—C3—C4	0.9 (3)	N1—C15—C16—C21	172.77 (15)
C1—C2—C3—C4	−177.09 (17)	N2—C15—C16—C17	171.79 (15)
C2—C3—C4—C5	−0.2 (3)	N1—C15—C16—C17	−8.2 (3)
C3—C4—C5—C6	−0.4 (3)	C21—C16—C17—C18	−1.2 (3)
C4—C5—C6—C7	0.2 (3)	C15—C16—C17—C18	179.86 (16)
C5—C6—C7—C2	0.6 (3)	C16—C17—C18—C19	−0.1 (3)
C5—C6—C7—C8	178.84 (18)	C17—C18—C19—C20	1.2 (3)
C3—C2—C7—C6	−1.1 (2)	C17—C18—C19—C22	−177.10 (18)
C1—C2—C7—C6	177.11 (15)	C18—C19—C20—C21	−1.1 (3)
C3—C2—C7—C8	−179.34 (15)	C22—C19—C20—C21	177.20 (17)
C1—C2—C7—C8	−1.2 (2)	C19—C20—C21—C16	−0.1 (3)
C6—C7—C8—C13	−174.43 (15)	C17—C16—C21—C20	1.3 (3)
C2—C7—C8—C13	3.8 (2)	C15—C16—C21—C20	−179.66 (16)
C6—C7—C8—C9	6.1 (2)	C18—C19—C22—F3	80.8 (2)
C2—C7—C8—C9	−175.70 (15)	C20—C19—C22—F3	−97.5 (2)
C13—C8—C9—C10	0.7 (3)	C18—C19—C22—F2	−159.34 (18)
C7—C8—C9—C10	−179.85 (17)	C20—C19—C22—F2	22.4 (3)
C8—C9—C10—C11	0.3 (3)	C18—C19—C22—F1	−38.2 (3)
C9—C10—C11—C12	−0.6 (3)	C20—C19—C22—F1	143.46 (19)
C10—C11—C12—C13	−0.2 (3)	C15—N1—C23—C28	92.07 (19)
C11—C12—C13—C8	1.3 (3)	C1—N1—C23—C28	−86.95 (19)
C11—C12—C13—C14	−176.70 (16)	C15—N1—C23—C24	−87.77 (19)
C9—C8—C13—C12	−1.5 (2)	C1—N1—C23—C24	93.20 (18)
C7—C8—C13—C12	179.04 (15)	C28—C23—C24—C25	−1.0 (2)
C9—C8—C13—C14	176.61 (14)	N1—C23—C24—C25	178.82 (14)
C7—C8—C13—C14	−2.9 (2)	C23—C24—C25—C26	0.5 (3)
C15—N2—C14—C1	−0.67 (17)	C29—O1—C26—C25	−175.49 (19)
C15—N2—C14—C13	177.31 (14)	C29—O1—C26—C27	4.5 (3)
N1—C1—C14—N2	0.23 (17)	C24—C25—C26—O1	−179.80 (15)
C2—C1—C14—N2	−178.74 (13)	C24—C25—C26—C27	0.2 (3)
N1—C1—C14—C13	−177.86 (13)	O1—C26—C27—C28	179.47 (16)
C2—C1—C14—C13	3.2 (2)	C25—C26—C27—C28	−0.6 (3)

C12—C13—C14—N2	−0.2 (2)	C24—C23—C28—C27	0.7 (2)
C8—C13—C14—N2	−178.24 (15)	N1—C23—C28—C27	−179.15 (15)
C12—C13—C14—C1	177.59 (15)	C26—C27—C28—C23	0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C28—H28···N2^{i}	0.95	2.55	3.402 (2)	150
C3—H3···*Cg*1	0.95	2.86	3.719 (2)	154
C10—H10···*Cg*2^{ii}	0.95	2.69	3.419 (2)	136
C17—H17···*Cg*1	0.95	2.74	3.6042 (2)	154

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