



Intra- and intermolecular C—H···F hydrogen bonds in the crystal structure of 1,2-bis[2-(2,3,4,5-tetrafluorophenyl)ethynyl]benzene

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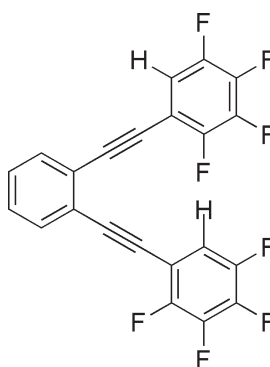
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The title molecule, C₂₂H₆F₈, crystallizes in the monoclinic space group *P*2₁/*c* with two unique molecules in the asymmetric unit and *Z* = 8. Each molecule features a short intramolecular *sp*²-C—H···F hydrogen bond with H···F separations at 2.363 (14) and 2.270 (14) Å, corresponding to 91 and 87.5% of the sum of the van der Waals radii, and C—H···F angles of 158.3 (14) and 166.8 (14)°, respectively. Each molecule also forms an intermolecular bifurcated CH···(F)₂ interaction with H···F distances ranging from 2.500 (16) to 2.597 (17) Å.

1. Chemical context

Non-covalent interactions, including hydrogen bonding, halogen bonding and coordinate bonds, are incorporated in the design and deliberate formation of multicomponent supramolecular solids with desired physical properties (Panja & Adams, 2021). Amongst hydrogen bonds, the existence of C—H hydrogen bonds to O and N has long been recognized and extensively reviewed (Desiraju, 1991). The focus of this report is the lesser-known C—H···F hydrogen bond. The role of organic fluorine as a C—H hydrogen-bond acceptor, while controversial, is now accepted to be a weak interaction (Cole & Taylor, 2022). The title compound, 1,2-*bis*-(2,3,4,5-tetrafluorophenylethynyl) benzene, was specifically prepared to probe intramolecular C—H···F hydrogen bonding. We had previously used the same framework to demonstrate intramolecular halogen bonding (Widner *et al.*, 2014) and intramolecular C—H···N hydrogen bonding (Bosch *et al.*, 2015).



2. Structural commentary

The compound C₂₂H₆F₈ crystallizes in the monoclinic space group *P*2₁/*c* with two unique molecules in the asymmetric unit.

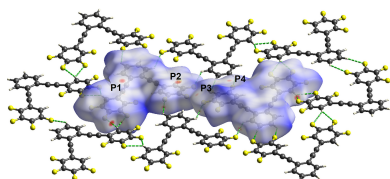


Table 1
Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ... <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> — <i>H</i> ... <i>A</i>
C5—H5...F5	0.98 (1)	2.27 (1)	3.230 (2)	167 (1)
C44—H44...F14 ⁱ	0.95 (1)	2.57 (2)	3.356 (2)	140 (1)
C44—H44...F15 ⁱ	0.95 (1)	2.46 (2)	3.314 (2)	150 (1)
C27—H27...F13	0.96 (1)	2.36 (1)	3.278 (2)	158 (1)
C22—H22...F6 ⁱⁱ	0.95 (2)	2.60 (2)	3.389 (2)	141 (2)
C22—H22...F7 ⁱⁱ	0.95 (2)	2.50 (2)	3.345 (2)	148 (2)

Symmetry codes: (i) $-x + 1, y - \frac{1}{2}, -z - \frac{1}{2}$; (ii) $-x + 2, y + \frac{1}{2}, -z + \frac{5}{2}$.

In each molecule, as shown in Fig. 1, an H atom on one tetrafluorophenyl ring forms an intramolecular hydrogen bond to an F atom on the second tetrafluorophenyl ring. The intermolecular dihedral angle between the two core benzene rings, C1–C6 and C23–C28, is 5.34 (6)°. The intramolecular C—H...F hydrogen bonds (Table 1) have separations H5...F5 and H27...F13 of 2.270 (14) and 2.363 (14) Å and C—H...F angles of 166.8 (14) and 158.3 (14)°, respectively. These separations are 87.5 and 91.0% of the sum of the van der Waals radii (Bondi, 1964).

The two unique molecules are essentially planar and coplanar in the crystal structure. The intramolecularly hydrogen-bonded tetrafluorophenyl rings are slightly twisted with respect to the central diethynyl benzene ring. The intramolecular dihedral angles between tetrafluoro phenyl rings that are C—H...F hydrogen bonded are 13.01 (6)° between benzene rings C1–C6 and C17–C22 and 9.63 (6)° between benzene rings C23–C28 and C39–C44. The F...F contacts between the adjacent molecules in the asymmetric unit are 3.0900 (15), 3.1719 (15) and 3.0223 (15) Å for F3...F10, F2...F11 and F3...F11, respectively. These separations are above the sum of the van der Waals radii of 2.80 Å.

3. Supramolecular features

The two hydrogen atoms on the tetrafluorophenyl rings that are not involved in intramolecular hydrogen bonding (Table 1) each have close contacts with two fluorine atoms on adjacent tetrafluorophenyl rings labelled as 'x' and 'y' in Fig. 2. The H...F separations in 'x', H22...F6ⁱ and H22...F7ⁱ, are

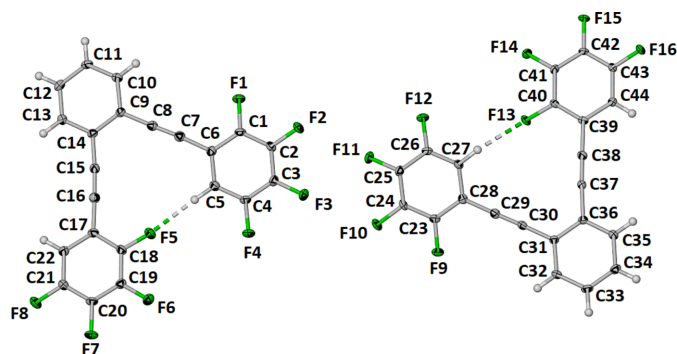


Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level and the intramolecular C—H...F hydrogen bonds shown as dashed lines.

2.597 (17) and 2.500 (16) Å, respectively [symmetry code: (i) $1 - x, y - \frac{1}{2}, -z - \frac{1}{2}$] and those in 'y', H44...F14ⁱⁱ and H44...F15ⁱⁱ, are 2.574 (16) and 2.460 (15) Å, respectively [symmetry code: (ii) $2 - x, \frac{1}{2} + y, \frac{5}{2} - z$].

The non-covalent interactions were investigated and visualized using Hirshfeld surface analysis (Spackman *et al.*, 2021) as shown in Fig. 3. The red spots on the Hirshfeld surface represent close contacts with separations less than the sum of the van der Waals radii while the dark-blue areas correspond to areas where the separations are greater than the sum of the van der Waals radii. The red areas in the plane of the molecules correspond to C—H...F hydrogen bonds with the hydrogen-bonded molecules shown.

Also shown in this figure are several close contacts corresponding to π -stacking; labelled **P1–P4**. Contacts **P1** and **P2** correspond to interactions between an alkynyl C atom and a tetrafluorophenyl C atom. The separations for C38...C25ⁱ and C25...C8ⁱ are 3.282 (3) and 3.273 (3) Å respectively [symmetry code: (i) $x, -y + \frac{3}{2}, z - \frac{1}{2}$]. Contact **P3** is between an F atom and a tetrafluorophenyl H atom while contact **P4** is between two tetrafluoro phenyl C atoms. The separations are 2.874 (16) and 3.321 (3) Å for F2...H5ⁱⁱ and C4...C19ⁱⁱ, respectively [symmetry code: (ii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$]. The planar sheets are π -stacked along the *b*-axis direction as shown in Fig. 4.

The fingerprint plots of the close contacts revealed on the surface of each individual molecule in the asymmetric unit are shown in Fig. 5 along with the corresponding percentage of the surface area. In both molecules, the dominant interaction is F...H and is largely between adjacent molecules in the same plane. Within each fingerprint plot, the interactions with higher frequency are colored turquoise through green, yellow and red with red corresponding to the highest frequency. The C...C interaction that is exclusively correlated to interactions between π -stacked molecules has a high frequency of interactions focused on distances d_i and d_e of 1.8 Å corresponding to a π – π separation of 3.6 Å, typical for π -stacking.

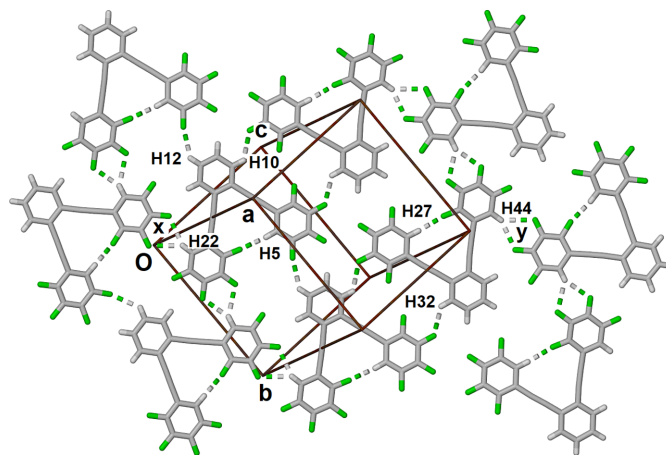


Figure 2

Partial view of one sheet of molecules in the crystal structure with bifurcated C—H...F interactions labeled 'x' and 'y'.

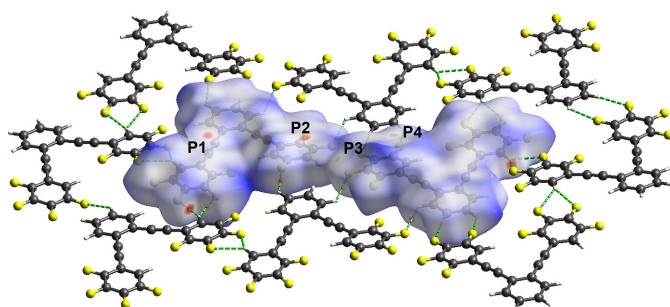


Figure 3

Hirshfeld surface for both molecules in the asymmetric unit with d_{norm} mapped over the surface. Included are the molecules within the same plane separated by less than 3.25 Å with C—H...F hydrogen bonds shown as green dashed lines. Close contacts related to π -stacked molecules are labelled **P1** to **P4** (see text).

4. Database survey

A search of the Cambridge Structural Database (CSD2024.2.0, build 415171; Groom *et al.*, 2016) for C—H...F contacts between an aryl H and an aryl F atom with an H...F separation less than or equal to the sum of the van der Waals radii with the C—F...H angle between 90 and 180° was performed. The search was further limited to single-crystal structures of organic compounds with 3D coordinates determined, *R* factor less than or equal to 0.1, only non-disordered, non polymeric structures with no errors. This search yielded 7195 unique database entries, including duplicate structures and structures at multiple temperatures, for a total of 13,732 data points. Most of these data points (10,370) have H...F separations greater than 2.5 Å, as shown in Fig. 6. The shorter separations are mostly found within sterically constrained environments. For example, in the structure of 1,2,4-trifluoro-3-phenyltriphenylene, an H—F separation of 2.018 Å, 77.6% of the sum of the van der Waals radii, is observed. This interaction corresponds to a 1,6 H...F interaction between atoms on adjacent phenyl rings in the planar triphenylene core of 1,2,4-trifluoro-3-phenyltriphenylene (Pan *et al.*, 2023). This is an example of a sterically induced/enforced short intramolecular interaction. Similar, very short intermolecular

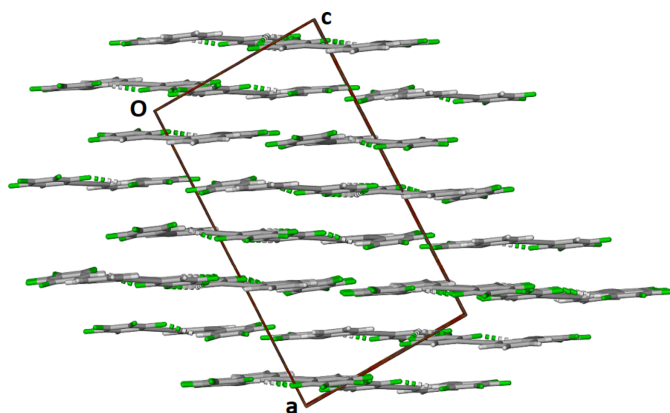


Figure 4

Partial view of the packing within the crystal structure along the *b*-axis.

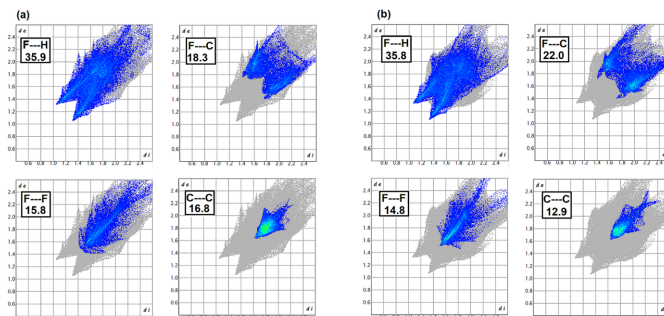


Figure 5

The two-dimensional fingerprint plots delineated into F...H contacts, F...C contacts, F...F contacts and C...C contacts for each of the individual molecules in the asymmetric unit along with the relative percentages. In all cases, reciprocal contacts are included.

separations are reported for co-crystals containing anthracene and octafluoronaphthalene with data collected under pressure (Friedrich *et al.*, 2020). Thus, at 120 K and atmospheric pressure the shortest C—H...F contact is 2.481 Å (Collings *et al.* 2001), while under a pressure of 22.2 GPa at 293 K this separation is reduced to 1.944 Å.

5. Synthesis and crystallization

The title compound, C₂₂H₆F₈, as prepared by palladium-catalyzed Sonogashira coupling of 1,2,3,4-tetrafluoro-5-iodobenzene and 1,2-diethynylbenzene. 1,2-Diethynylbenzene was prepared from 1,2-diiodobenzene as previously described (Takahashi *et al.*, 1980) while all other chemicals were commercially available and used as received. 1,2-Diethynylbenzene (0.22 g, 1.7 mmol) and 1,2,3,4-tetrafluoro-5-iodobenzene (0.88 g, 3.8 mmol) were dissolved in NEt₃ (4 mL) in a pressure flask. Argon was bubbled through the solution for 10 minutes and PdCl₂(PPh₃)₂ (50 mg, 0.06 mmol) and CuI (25 mg, 0.12 mmol) then added to the flask. The flask was sealed and stirred at 333 K for 24 h. The solvent was evaporated from the crude reaction mixture and the residue purified using flash column chromatography with progressively more

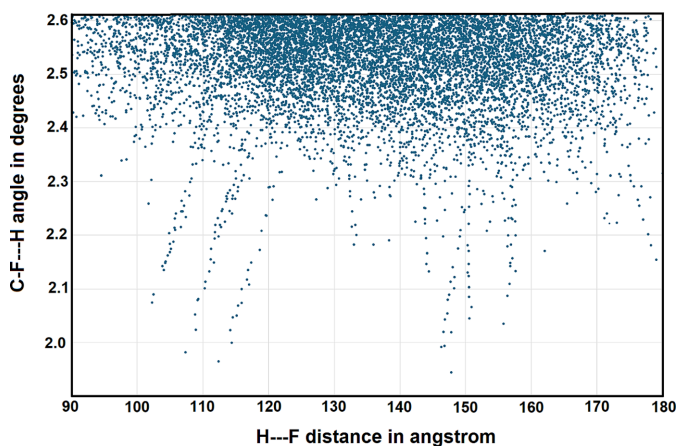


Figure 6

Scatter plot of the hydrogen-bond distance (H...F) versus the C—F...H bond angle for single-crystal X-ray structures deposited in the CSD.

polar mixtures of hexane and ethyl acetate to give the title compound as colorless crystals (0.43 g, 59%). Crystals suitable for single-crystal X-ray diffraction were grown on slow evaporation from a dichloromethane solution.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were located in difference maps. H atoms involved in C—H...F hydrogen-bonding interactions were restrained in the refinement with C—H = 0.95 (2) Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. All other H atoms were treated as riding atoms in geometrically idealized positions with C—H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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Table 2

Experimental details.

Crystal data	
Chemical formula	C ₂₂ H ₆ F ₈
M_r	422.27
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	21.8447 (13), 13.0140 (8), 12.1123 (7)
β (°)	92.620 (1)
V (Å ³)	3439.8 (4)
Z	8
Radiation type	Mo $K\alpha$
μ (mm ^{−1})	0.16
Crystal size (mm)	0.25 × 0.25 × 0.15
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.672, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	44014, 7632, 5101
R_{int}	0.048
$(\sin \theta/\lambda)_{\text{max}}$ (Å ^{−1})	0.642
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.040, 0.111, 1.01
No. of reflections	7632
No. of parameters	557
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ^{−3})	0.23, −0.29

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), and *X-SEED* (Barbour, 2020).

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Intra- and intermolecular C—H $\cdots$ F hydrogen bonds in the crystal structure of 1,2-bis[2-(2,3,4,5-tetrafluorophenyl)ethynyl]benzene

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Computing details

1,2-Bis[2-(2,3,4,5-tetrafluorophenyl)ethynyl]benzene

Crystal data

C₂₂H₆F₈

$M_r = 422.27$

Monoclinic, $P2_1/c$

$a = 21.8447$ (13) Å

$b = 13.0140$ (8) Å

$c = 12.1123$ (7) Å

$\beta = 92.620$ (1)°

$V = 3439.8$ (4) Å³

$Z = 8$

$F(000) = 1680$

$D_x = 1.631$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 7323 reflections

$\theta = 2.3\text{--}27.1^\circ$

$\mu = 0.16$ mm⁻¹

$T = 100$ K

Block, colourless

$0.25 \times 0.25 \times 0.15$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3660 pixels mm⁻¹

phi and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.672$, $T_{\max} = 0.746$

44014 measured reflections

7632 independent reflections

5101 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 27.2^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -28 \rightarrow 28$

$k = -16 \rightarrow 16$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.111$

$S = 1.01$

7632 reflections

557 parameters

4 restraints

Primary atom site location: dual

Secondary atom site location: diffmap

Hydrogen site location: mixed

H atoms treated by a mixture of independent

and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0515P)^2 + 1.115P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.23$ e Å⁻³

$\Delta\rho_{\min} = -0.29$ 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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.77779 (5)	0.93658 (8)	0.51579 (9)	0.0338 (3)
C1	0.79548 (8)	0.86262 (14)	0.58746 (14)	0.0214 (4)
F2	0.75740 (5)	0.73905 (9)	0.45920 (8)	0.0314 (3)
C2	0.78455 (8)	0.76168 (14)	0.55770 (14)	0.0212 (4)
F3	0.79008 (5)	0.58519 (8)	0.60076 (9)	0.0298 (3)
C3	0.80089 (8)	0.68326 (14)	0.62972 (15)	0.0218 (4)
F4	0.84323 (5)	0.63004 (8)	0.80143 (9)	0.0340 (3)
C4	0.82795 (8)	0.70779 (14)	0.73179 (15)	0.0227 (4)
F5	0.92433 (5)	0.84712 (8)	0.98359 (9)	0.0322 (3)
C5	0.83980 (8)	0.80741 (14)	0.76191 (15)	0.0235 (4)
F6	0.97196 (5)	0.70715 (8)	1.12628 (9)	0.0321 (3)
C6	0.82350 (8)	0.88797 (14)	0.68959 (14)	0.0207 (4)
F7	1.01924 (5)	0.76616 (9)	1.32791 (9)	0.0320 (3)
C7	0.83445 (8)	0.99237 (15)	0.72119 (15)	0.0233 (4)
F8	1.01963 (5)	0.96706 (9)	1.38461 (9)	0.0367 (3)
C8	0.84329 (8)	1.07804 (14)	0.75469 (15)	0.0216 (4)
F9	0.71615 (5)	0.16630 (8)	0.47865 (8)	0.0280 (3)
C9	0.84968 (8)	1.18143 (13)	0.79439 (14)	0.0192 (4)
F10	0.74191 (5)	0.36203 (8)	0.53715 (8)	0.0291 (3)
C10	0.82886 (8)	1.26325 (14)	0.72793 (15)	0.0215 (4)
H10	0.812171	1.250130	0.655498	0.026*
F11	0.72140 (5)	0.51762 (8)	0.39096 (9)	0.0273 (3)
C11	0.83237 (8)	1.36323 (14)	0.76679 (15)	0.0229 (4)
H11	0.817786	1.418206	0.721180	0.027*
F12	0.67428 (5)	0.47675 (8)	0.18546 (9)	0.0314 (3)
C12	0.85710 (8)	1.38342 (14)	0.87206 (15)	0.0245 (4)
H12	0.859125	1.452112	0.898504	0.029*
F13	0.57293 (5)	0.25053 (8)	0.01742 (8)	0.0246 (2)
C13	0.87890 (8)	1.30360 (14)	0.93890 (15)	0.0225 (4)
H13	0.896161	1.318106	1.010618	0.027*
F14	0.52464 (5)	0.39200 (8)	−0.12408 (8)	0.0275 (3)
C14	0.87566 (8)	1.20176 (14)	0.90146 (15)	0.0199 (4)
F15	0.47673 (5)	0.33454 (8)	−0.32557 (8)	0.0269 (3)
C15	0.89857 (8)	1.12068 (14)	0.97172 (14)	0.0212 (4)
F16	0.47389 (5)	0.13386 (8)	−0.38270 (8)	0.0274 (3)
C16	0.91961 (8)	1.05709 (14)	1.03384 (15)	0.0230 (4)
C17	0.94577 (8)	0.98316 (14)	1.11011 (15)	0.0210 (4)
C18	0.94714 (8)	0.87951 (14)	1.08257 (14)	0.0220 (4)
C19	0.97165 (8)	0.80652 (14)	1.15475 (15)	0.0226 (4)

C20	0.99584 (8)	0.83679 (14)	1.25661 (15)	0.0234 (4)
C21	0.99569 (8)	0.94005 (15)	1.28511 (15)	0.0243 (4)
C22	0.97135 (8)	1.01266 (15)	1.21354 (15)	0.0231 (4)
C23	0.70518 (8)	0.24157 (14)	0.40448 (14)	0.0192 (4)
C24	0.71860 (8)	0.34157 (14)	0.43517 (14)	0.0198 (4)
C25	0.70821 (8)	0.42049 (14)	0.36111 (15)	0.0204 (4)
C26	0.68407 (8)	0.39796 (14)	0.25635 (14)	0.0205 (4)
C27	0.67024 (8)	0.29921 (14)	0.22483 (14)	0.0195 (4)
C28	0.68050 (8)	0.21840 (14)	0.29938 (14)	0.0189 (4)
C29	0.66737 (8)	0.11407 (14)	0.26837 (14)	0.0204 (4)
C30	0.65718 (8)	0.02747 (14)	0.23943 (14)	0.0198 (4)
C31	0.64841 (7)	−0.07709 (13)	0.20536 (14)	0.0177 (4)
C32	0.66839 (8)	−0.15734 (14)	0.27533 (15)	0.0222 (4)
H32	0.686437	−0.141961	0.346255	0.027*
C33	0.66212 (8)	−0.25874 (14)	0.24218 (15)	0.0238 (4)
H33	0.675455	−0.312447	0.290666	0.029*
C34	0.63633 (8)	−0.28225 (14)	0.13805 (16)	0.0241 (4)
H34	0.632677	−0.351878	0.115140	0.029*
C35	0.61592 (8)	−0.20398 (14)	0.06754 (15)	0.0205 (4)
H35	0.598433	−0.220417	−0.003519	0.025*
C36	0.62093 (7)	−0.10131 (13)	0.10035 (14)	0.0179 (4)
C37	0.59700 (8)	−0.02175 (13)	0.02839 (14)	0.0181 (4)
C38	0.57445 (8)	0.04127 (14)	−0.03304 (14)	0.0195 (4)
C39	0.54855 (7)	0.11567 (13)	−0.10834 (14)	0.0176 (4)
C40	0.54873 (7)	0.21924 (13)	−0.08080 (13)	0.0176 (4)
C41	0.52474 (8)	0.29280 (13)	−0.15302 (14)	0.0191 (4)
C42	0.50012 (8)	0.26319 (13)	−0.25523 (14)	0.0195 (4)
C43	0.49908 (8)	0.16028 (13)	−0.28360 (14)	0.0194 (4)
C44	0.52294 (8)	0.08682 (14)	−0.21200 (15)	0.0200 (4)
H5	0.8594 (7)	0.8242 (13)	0.8339 (12)	0.015 (4)*
H44	0.5228 (8)	0.0162 (11)	−0.2305 (14)	0.018 (5)*
H27	0.6514 (7)	0.2864 (13)	0.1527 (12)	0.014 (4)*
H22	0.9727 (8)	1.0835 (12)	1.2336 (16)	0.026 (5)*

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0503 (7)	0.0241 (6)	0.0262 (6)	0.0040 (5)	−0.0059 (5)	0.0067 (5)
C1	0.0253 (10)	0.0191 (9)	0.0195 (9)	0.0047 (7)	−0.0006 (7)	0.0053 (7)
F2	0.0432 (7)	0.0315 (6)	0.0186 (6)	0.0005 (5)	−0.0095 (5)	−0.0030 (5)
C2	0.0226 (9)	0.0255 (10)	0.0154 (9)	0.0020 (7)	−0.0022 (7)	−0.0020 (7)
F3	0.0379 (6)	0.0175 (6)	0.0334 (6)	−0.0002 (5)	−0.0056 (5)	−0.0036 (5)
C3	0.0235 (9)	0.0167 (9)	0.0252 (10)	0.0004 (7)	0.0008 (7)	−0.0035 (7)
F4	0.0479 (7)	0.0234 (6)	0.0295 (6)	0.0036 (5)	−0.0115 (5)	0.0081 (5)
C4	0.0266 (10)	0.0186 (10)	0.0226 (9)	0.0046 (7)	−0.0027 (7)	0.0048 (8)
F5	0.0398 (7)	0.0300 (6)	0.0255 (6)	0.0037 (5)	−0.0113 (5)	−0.0024 (5)
C5	0.0250 (10)	0.0238 (10)	0.0212 (10)	0.0022 (8)	−0.0030 (8)	−0.0010 (8)
F6	0.0379 (7)	0.0192 (6)	0.0384 (7)	0.0034 (5)	−0.0070 (5)	−0.0005 (5)

C6	0.0217 (9)	0.0185 (9)	0.0220 (9)	0.0015 (7)	0.0020 (7)	−0.0014 (7)
F7	0.0364 (6)	0.0286 (6)	0.0301 (6)	0.0063 (5)	−0.0084 (5)	0.0103 (5)
C7	0.0233 (10)	0.0234 (10)	0.0231 (10)	0.0021 (7)	0.0007 (7)	0.0001 (8)
F8	0.0482 (7)	0.0361 (7)	0.0244 (6)	0.0038 (6)	−0.0141 (5)	−0.0029 (5)
C8	0.0215 (9)	0.0220 (10)	0.0211 (9)	0.0020 (7)	0.0011 (7)	0.0014 (8)
F9	0.0400 (7)	0.0231 (6)	0.0207 (6)	0.0033 (5)	−0.0024 (5)	0.0060 (4)
C9	0.0175 (8)	0.0174 (9)	0.0227 (9)	−0.0001 (7)	0.0008 (7)	0.0011 (7)
F10	0.0370 (6)	0.0323 (6)	0.0172 (5)	0.0008 (5)	−0.0077 (5)	−0.0052 (5)
C10	0.0204 (9)	0.0237 (10)	0.0203 (9)	0.0008 (7)	−0.0002 (7)	0.0034 (8)
F11	0.0329 (6)	0.0173 (6)	0.0313 (6)	−0.0022 (4)	−0.0020 (5)	−0.0053 (5)
C11	0.0228 (9)	0.0191 (9)	0.0267 (10)	0.0023 (7)	0.0006 (7)	0.0070 (8)
F12	0.0454 (7)	0.0208 (6)	0.0272 (6)	0.0037 (5)	−0.0070 (5)	0.0072 (5)
C12	0.0268 (10)	0.0167 (9)	0.0301 (10)	−0.0009 (7)	0.0034 (8)	0.0010 (8)
F13	0.0309 (6)	0.0263 (6)	0.0157 (5)	0.0022 (4)	−0.0079 (4)	−0.0021 (4)
C13	0.0233 (9)	0.0224 (10)	0.0216 (10)	−0.0013 (7)	−0.0014 (7)	−0.0009 (8)
F14	0.0409 (7)	0.0160 (5)	0.0249 (6)	0.0038 (5)	−0.0063 (5)	−0.0018 (4)
C14	0.0175 (8)	0.0188 (9)	0.0233 (9)	−0.0006 (7)	0.0008 (7)	0.0040 (7)
F15	0.0367 (6)	0.0211 (6)	0.0218 (6)	0.0040 (5)	−0.0093 (5)	0.0074 (4)
C15	0.0211 (9)	0.0211 (10)	0.0212 (9)	0.0003 (7)	−0.0005 (7)	−0.0005 (8)
F16	0.0377 (6)	0.0263 (6)	0.0171 (5)	−0.0037 (5)	−0.0113 (5)	0.0001 (4)
C16	0.0226 (9)	0.0232 (10)	0.0232 (10)	0.0005 (8)	0.0011 (7)	0.0003 (8)
C17	0.0189 (9)	0.0205 (9)	0.0236 (9)	0.0020 (7)	−0.0004 (7)	0.0042 (8)
C18	0.0205 (9)	0.0249 (10)	0.0203 (9)	0.0005 (7)	−0.0031 (7)	0.0017 (8)
C19	0.0217 (9)	0.0177 (9)	0.0283 (10)	0.0031 (7)	−0.0013 (7)	0.0008 (8)
C20	0.0214 (9)	0.0236 (10)	0.0248 (10)	0.0041 (7)	−0.0025 (7)	0.0077 (8)
C21	0.0255 (10)	0.0259 (10)	0.0211 (9)	−0.0003 (8)	−0.0038 (7)	−0.0001 (8)
C22	0.0240 (10)	0.0201 (10)	0.0249 (10)	0.0009 (7)	−0.0011 (8)	0.0010 (8)
C23	0.0198 (9)	0.0202 (10)	0.0176 (9)	0.0037 (7)	0.0010 (7)	0.0030 (7)
C24	0.0193 (9)	0.0251 (10)	0.0145 (8)	0.0005 (7)	−0.0030 (7)	−0.0037 (7)
C25	0.0225 (9)	0.0156 (9)	0.0231 (9)	0.0003 (7)	0.0004 (7)	−0.0035 (7)
C26	0.0225 (9)	0.0201 (9)	0.0188 (9)	0.0032 (7)	−0.0010 (7)	0.0050 (7)
C27	0.0210 (9)	0.0213 (10)	0.0158 (9)	0.0015 (7)	−0.0027 (7)	−0.0010 (7)
C28	0.0179 (8)	0.0203 (9)	0.0185 (9)	0.0010 (7)	0.0020 (7)	−0.0021 (7)
C29	0.0197 (9)	0.0225 (10)	0.0190 (9)	0.0014 (7)	−0.0001 (7)	−0.0005 (8)
C30	0.0195 (9)	0.0231 (10)	0.0163 (9)	0.0006 (7)	−0.0023 (7)	0.0015 (7)
C31	0.0174 (8)	0.0168 (9)	0.0187 (9)	0.0007 (7)	−0.0006 (7)	0.0021 (7)
C32	0.0237 (9)	0.0230 (10)	0.0193 (9)	0.0020 (7)	−0.0047 (7)	0.0032 (8)
C33	0.0237 (9)	0.0197 (10)	0.0276 (10)	0.0024 (7)	−0.0030 (8)	0.0088 (8)
C34	0.0249 (10)	0.0165 (9)	0.0307 (10)	0.0023 (7)	−0.0025 (8)	0.0019 (8)
C35	0.0206 (9)	0.0217 (10)	0.0191 (9)	0.0000 (7)	−0.0025 (7)	0.0002 (7)
C36	0.0166 (8)	0.0182 (9)	0.0190 (9)	−0.0004 (7)	0.0002 (7)	0.0035 (7)
C37	0.0191 (9)	0.0179 (9)	0.0170 (9)	−0.0007 (7)	−0.0016 (7)	−0.0006 (7)
C38	0.0187 (9)	0.0215 (10)	0.0182 (9)	−0.0005 (7)	−0.0007 (7)	0.0012 (7)
C39	0.0148 (8)	0.0211 (9)	0.0170 (9)	0.0001 (7)	0.0002 (7)	0.0047 (7)
C40	0.0187 (9)	0.0208 (9)	0.0130 (8)	0.0004 (7)	−0.0027 (7)	0.0012 (7)
C41	0.0220 (9)	0.0134 (9)	0.0219 (9)	0.0004 (7)	−0.0007 (7)	−0.0004 (7)
C42	0.0227 (9)	0.0180 (9)	0.0173 (9)	0.0011 (7)	−0.0043 (7)	0.0066 (7)
C43	0.0228 (9)	0.0197 (9)	0.0153 (8)	−0.0026 (7)	−0.0044 (7)	0.0002 (7)

C44	0.0227 (9)	0.0174 (9)	0.0195 (9)	−0.0027 (7)	−0.0029 (7)	0.0015 (7)
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Geometric parameters (Å, °)

F1—C1	1.341 (2)	C16—C17	1.434 (2)
C1—C2	1.380 (3)	C17—C18	1.390 (3)
C1—C6	1.394 (2)	C17—C22	1.402 (3)
F2—C2	1.341 (2)	C18—C19	1.382 (2)
C2—C3	1.379 (3)	C19—C20	1.377 (3)
F3—C3	1.342 (2)	C20—C21	1.387 (3)
C3—C4	1.383 (3)	C21—C22	1.373 (3)
F4—C4	1.349 (2)	C22—H22	0.953 (15)
C4—C5	1.368 (3)	C23—C24	1.381 (2)
F5—C18	1.345 (2)	C23—C28	1.393 (2)
C5—C6	1.402 (3)	C24—C25	1.376 (2)
C5—H5	0.978 (13)	C25—C26	1.383 (2)
F6—C19	1.339 (2)	C26—C27	1.370 (2)
C6—C7	1.429 (3)	C27—C28	1.398 (2)
F7—C20	1.346 (2)	C27—H27	0.963 (13)
C7—C8	1.199 (3)	C28—C29	1.434 (3)
F8—C21	1.339 (2)	C29—C30	1.198 (2)
C8—C9	1.433 (3)	C30—C31	1.432 (2)
F9—C23	1.3433 (19)	C31—C32	1.402 (2)
C9—C10	1.398 (2)	C31—C36	1.417 (2)
C9—C14	1.417 (2)	C32—C33	1.384 (3)
F10—C24	1.3411 (19)	C32—H32	0.9500
C10—C11	1.385 (3)	C33—C34	1.392 (3)
C10—H10	0.9500	C33—H33	0.9500
F11—C25	1.342 (2)	C34—C35	1.389 (2)
C11—C12	1.387 (3)	C34—H34	0.9500
C11—H11	0.9500	C35—C36	1.397 (2)
F12—C26	1.3483 (19)	C35—H35	0.9500
C12—C13	1.388 (3)	C36—C37	1.437 (2)
C12—H12	0.9500	C37—C38	1.198 (2)
F13—C40	1.3429 (19)	C38—C39	1.429 (2)
C13—C14	1.401 (3)	C39—C40	1.388 (2)
C13—H13	0.9500	C39—C44	1.402 (2)
F14—C41	1.338 (2)	C40—C41	1.383 (2)
C14—C15	1.432 (2)	C41—C42	1.382 (2)
F15—C42	1.3451 (19)	C42—C43	1.383 (2)
C15—C16	1.196 (2)	C43—C44	1.377 (2)
F16—C43	1.3422 (19)	C44—H44	0.945 (14)
F1—C1—C2	118.22 (16)	F9—C23—C24	118.55 (15)
F1—C1—C6	120.41 (16)	F9—C23—C28	120.21 (16)
C2—C1—C6	121.37 (16)	C24—C23—C28	121.24 (16)
F2—C2—C3	119.45 (16)	F10—C24—C25	119.78 (16)
F2—C2—C1	120.37 (16)	F10—C24—C23	120.13 (16)

C3—C2—C1	120.18 (16)	C25—C24—C23	120.09 (16)
F3—C3—C2	120.09 (16)	F11—C25—C24	120.03 (15)
F3—C3—C4	121.07 (16)	F11—C25—C26	120.99 (16)
C2—C3—C4	118.84 (16)	C24—C25—C26	118.98 (16)
F4—C4—C5	120.36 (16)	F12—C26—C27	120.61 (16)
F4—C4—C3	117.97 (16)	F12—C26—C25	117.76 (16)
C5—C4—C3	121.66 (17)	C27—C26—C25	121.63 (16)
C4—C5—C6	120.17 (17)	C26—C27—C28	119.92 (16)
C4—C5—H5	121.2 (10)	C26—C27—H27	119.7 (11)
C6—C5—H5	118.6 (10)	C28—C27—H27	120.3 (11)
C1—C6—C5	117.78 (16)	C23—C28—C27	118.14 (16)
C1—C6—C7	121.60 (16)	C23—C28—C29	120.59 (16)
C5—C6—C7	120.61 (16)	C27—C28—C29	121.26 (16)
C8—C7—C6	175.7 (2)	C30—C29—C28	178.0 (2)
C7—C8—C9	176.33 (19)	C29—C30—C31	176.97 (19)
C10—C9—C14	119.40 (16)	C32—C31—C36	118.97 (16)
C10—C9—C8	119.84 (16)	C32—C31—C30	119.98 (16)
C14—C9—C8	120.75 (16)	C36—C31—C30	121.03 (15)
C11—C10—C9	120.56 (17)	C33—C32—C31	120.72 (16)
C11—C10—H10	119.7	C33—C32—H32	119.6
C9—C10—H10	119.7	C31—C32—H32	119.6
C10—C11—C12	120.24 (17)	C32—C33—C34	120.19 (16)
C10—C11—H11	119.9	C32—C33—H33	119.9
C12—C11—H11	119.9	C34—C33—H33	119.9
C11—C12—C13	120.22 (17)	C35—C34—C33	120.07 (17)
C11—C12—H12	119.9	C35—C34—H34	120.0
C13—C12—H12	119.9	C33—C34—H34	120.0
C12—C13—C14	120.54 (17)	C34—C35—C36	120.50 (16)
C12—C13—H13	119.7	C34—C35—H35	119.7
C14—C13—H13	119.7	C36—C35—H35	119.7
C13—C14—C9	119.01 (16)	C35—C36—C31	119.51 (15)
C13—C14—C15	119.58 (16)	C35—C36—C37	119.69 (15)
C9—C14—C15	121.41 (16)	C31—C36—C37	120.79 (16)
C16—C15—C14	176.2 (2)	C38—C37—C36	176.52 (19)
C15—C16—C17	178.3 (2)	C37—C38—C39	178.59 (19)
C18—C17—C22	117.91 (16)	C40—C39—C44	118.14 (15)
C18—C17—C16	120.57 (17)	C40—C39—C38	120.52 (15)
C22—C17—C16	121.51 (17)	C44—C39—C38	121.34 (16)
F5—C18—C19	117.74 (16)	F13—C40—C41	118.21 (15)
F5—C18—C17	120.46 (15)	F13—C40—C39	120.25 (15)
C19—C18—C17	121.80 (17)	C41—C40—C39	121.54 (15)
F6—C19—C20	120.05 (16)	F14—C41—C42	119.90 (15)
F6—C19—C18	120.49 (16)	F14—C41—C40	120.48 (15)
C20—C19—C18	119.46 (17)	C42—C41—C40	119.61 (16)
F7—C20—C19	119.90 (16)	F15—C42—C41	119.73 (15)
F7—C20—C21	120.46 (16)	F15—C42—C43	120.66 (15)
C19—C20—C21	119.65 (16)	C41—C42—C43	119.60 (15)
F8—C21—C22	120.78 (17)	F16—C43—C44	120.88 (16)

F8—C21—C20	118.23 (16)	F16—C43—C42	118.15 (15)
C22—C21—C20	120.98 (17)	C44—C43—C42	120.97 (16)
C21—C22—C17	120.18 (18)	C43—C44—C39	120.13 (17)
C21—C22—H22	119.9 (12)	C43—C44—H44	121.9 (11)
C17—C22—H22	119.9 (12)	C39—C44—H44	118.0 (11)

Hydrogen-bond geometry (Å, °)

<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>
C5—H5 $\cdots$ F5	0.98 (1)	2.27 (1)	3.230 (2)	167 (1)
C44—H44 $\cdots$ F14 ⁱ	0.95 (1)	2.57 (2)	3.356 (2)	140 (1)
C44—H44 $\cdots$ F15 ⁱ	0.95 (1)	2.46 (2)	3.314 (2)	150 (1)
C27—H27 $\cdots$ F13	0.96 (1)	2.36 (1)	3.278 (2)	158 (1)
C22—H22 $\cdots$ F6 ⁱⁱ	0.95 (2)	2.60 (2)	3.389 (2)	141 (2)
C22—H22 $\cdots$ F7 ⁱⁱ	0.95 (2)	2.50 (2)	3.345 (2)	148 (2)

Symmetry codes: (i) $-x+1, y-1/2, -z-1/2$; (ii) $-x+2, y+1/2, -z+5/2$.