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(Z)-1-(2,4-Difluorophenyl)-3-(4-fluorophenyl)-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one

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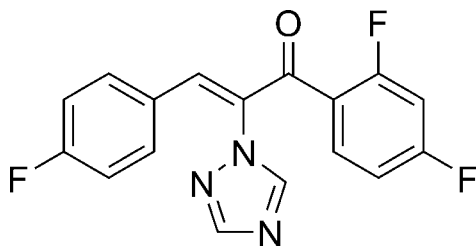
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.042; wR factor = 0.100; data-to-parameter ratio = 13.1.

In the title molecule, $\text{C}_{17}\text{H}_{10}\text{F}_3\text{N}_3\text{O}$, the $\text{C}=\text{C}$ bond connecting the triazole ring and 4-fluorophenyl groups adopts a Z conformation. The triazole ring forms dihedral angles of 15.3 (1) and 63.5 (1)°, with the 2,4-difluoro-substituted and 4-fluoro-substituted benzene rings, respectively. The dihedral angle between the two benzene rings is 51.8 (1)°.

Related literature

For the pharmacological activity of triazole derivatives, see: Wang & Zhou (2011); Zhou & Wang (2012). For the biological activity of chalcones, see: Jin *et al.* (2010). For related structures, see: Wang *et al.* (2009); Yan *et al.* (2009). For the synthesis, see: Yan *et al.* (2009).



Experimental

Crystal data

| | |
|--|-----------------------------------|
| $\text{C}_{17}\text{H}_{10}\text{F}_3\text{N}_3\text{O}$ | $V = 1444.4$ (12) Å ³ |
| $M_r = 329.28$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 11.735$ (6) Å | $\mu = 0.12$ mm ⁻¹ |
| $b = 7.698$ (4) Å | $T = 293$ K |
| $c = 17.065$ (7) Å | $0.19 \times 0.17 \times 0.16$ mm |
| $\beta = 110.45$ (3)° | |

Data collection

| | |
|--|--|
| Bruker APEXII CCD diffractometer | 7601 measured reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2009) | 2840 independent reflections |
| $T_{\min} = 0.977$, $T_{\max} = 0.980$ | 2095 reflections with $I > 2\sigma(I)$ |
| | $R_{\text{int}} = 0.027$ |

Refinement

| | |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | 217 parameters |
| $wR(F^2) = 0.100$ | H-atom parameters constrained |
| $S = 1.01$ | $\Delta\rho_{\text{max}} = 0.15$ e Å ⁻³ |
| 2840 reflections | $\Delta\rho_{\text{min}} = -0.21$ e Å ⁻³ |

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); 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: LH5435).

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supporting information

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(Z)-1-(2,4-Difluorophenyl)-3-(4-fluorophenyl)-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one**Ben-Tao Yin, Jing-Song Lv, Yan Wang and Cheng-He Zhou****S1. Comment**

Triazole compounds exhibit broad bioactive spectrum and the developments of new triazole derivatives as potential bioactive agents have become an active topic in medicinal chemistry (Wang & Zhou, 2011; Zhou & Wang, 2012). Chalcones have been paid increasingly special attention for their diverse biological activities such as antimicrobial, anticancer, antiviral and anti-inflammatory ones and so on (Jin *et al.*, 2010). Our interest is to develop novel triazole-derived chalcone compounds as medicinal agents. We have already synthesized and reported related structures of triazolylchalcones (Wang *et al.*, 2009; Yan *et al.*, 2009). Herein, we report the crystal structure of the title compound (I).

The molecular structure of (I) is shown in Fig. 1. The C=C bond connecting the triazole ring and 4-fluorophenyl groups adopts a *Z* geometry. The atoms in the region of the C=C bond have an essentially planar arrangement i.e. the r.m.s. deviation the atoms C7/C8/C11/C12/N1 is 0.0480 Å. The torsion angles of C12–C11=C8–C7 and C12–C11=C8–N1 are -169.35 (16)° and 7.1 (3)°. The triazole ring forms dihedral angles of 15.3 (1)° and 63.5 (1)°, with the 2,4-difluoro substituted (C1–C6) and 4-fluoro substituted (C12–C17) benzene rings, respectively. The dihedral angles between the two benzene rings is 51.8 (1)°.

S2. Experimental

Compound (I) was prepared according to the procedure of Yan *et al.* (2009). A mixture of 1-(2,4-difluorophenyl)-2-(1H-1,2,4-triazol-1-yl) ethanone (3.07 g, 13.8 mmol) and 4-fluorobenzaldehyde (1.89 g, 15.3 mmol) in toluene (30 mL) using glacial acetic acid (0.08 mL, 1.4 mmol) as catalyst was refluxed. After the reaction was complete (monitored by TLC, petroleum ether/ethyl acetate, 10/1, V/V), the solvent was removed. The residue was dissolved in dichloromethane (30 mL) and washed with water (3x30 mL). The resulting phase was dried over anhydrous sodium sulfate, concentrated under reduced pressure and then purified by silica gel column chromatography eluting with petroleum ether/ethyl acetate (10/1-2/1, V/V) to give the title compound (I) (2.578 g) as solid. Crystals suitable for X-ray analysis were grown from a mixed solution of (I) in ethyl acetate and petroleum ether by slow evaporation at room temperature.

S3. Refinement

H atoms were placed in calculated positions with C—H = 0.93 Å. The $U_{iso}(H)$ value was set equal to 1.2 $U_{eq}(C)$.

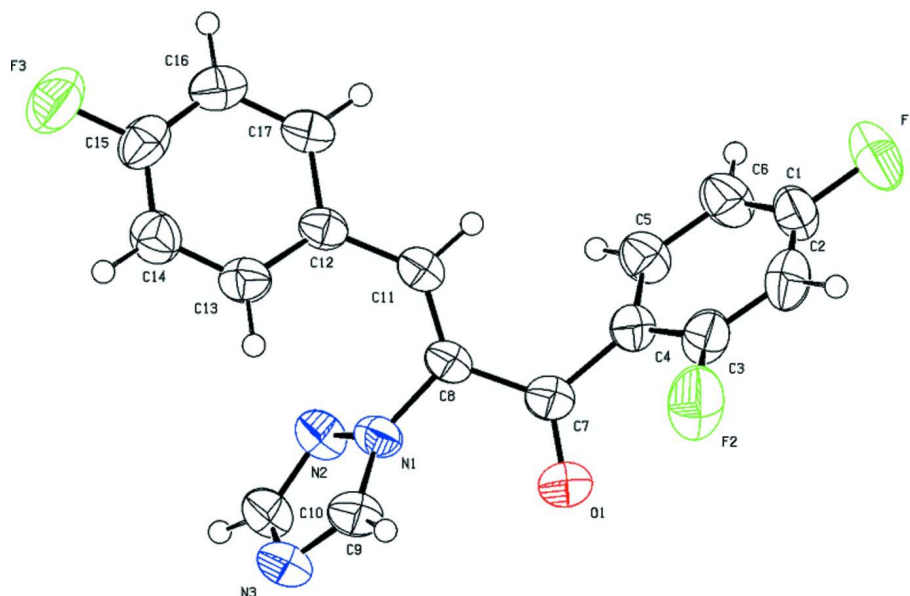


Figure 1

The molecular structure of (I), showing the displacement ellipsoids are drawn at the 50% probability level.

(Z)-1-(2,4-Difluorophenyl)-3-(4-fluorophenyl)-2-(1H-1,2,4-triazol-1-yl)prop-2-en-1-one

Crystal data

$C_{17}H_{10}F_3N_3O$

$M_r = 329.28$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 11.735$ (6) Å

$b = 7.698$ (4) Å

$c = 17.065$ (7) Å

$\beta = 110.45$ (3)°

$V = 1444.4$ (12) Å³

$Z = 4$

$F(000) = 672$

$D_x = 1.514$ Mg m⁻³

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

Cell parameters from 2158 reflections

$\theta = 2.9$ – 23.2 °

$\mu = 0.12$ mm⁻¹

$T = 293$ K

Block, colourless

$0.19 \times 0.17 \times 0.16$ mm

Data collection

Bruker APEXII CCD
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.977$, $T_{\max} = 0.980$

7601 measured reflections

2840 independent reflections

2095 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 26.0$ °, $\theta_{\min} = 2.6$ °

$h = -14 \rightarrow 14$

$k = -9 \rightarrow 9$

$l = -21 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.100$

$S = 1.01$

2840 reflections

217 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

$$w = 1/[\sigma^2(F_o^2) + (0.0398P)^2 + 0.3484P]$$

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

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

$$\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$$

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 $F^2 > \sigma(F^2)$ 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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|--------------|--------------|----------------------------------|
| F1 | -0.10204 (11) | 0.63601 (19) | 0.88238 (9) | 0.0882 (4) |
| F2 | 0.09918 (11) | 0.6680 (2) | 0.69415 (7) | 0.0836 (4) |
| F3 | 0.87808 (11) | 1.03042 (17) | 1.09542 (8) | 0.0816 (4) |
| O1 | 0.29519 (13) | 0.4323 (2) | 0.74119 (9) | 0.0862 (5) |
| N1 | 0.52550 (12) | 0.49839 (18) | 0.83262 (8) | 0.0416 (3) |
| N2 | 0.61373 (13) | 0.40221 (19) | 0.88775 (9) | 0.0498 (4) |
| N3 | 0.64451 (15) | 0.4248 (2) | 0.76604 (10) | 0.0619 (5) |
| C1 | -0.00130 (16) | 0.6098 (3) | 0.86429 (13) | 0.0551 (5) |
| C2 | -0.00402 (16) | 0.6532 (3) | 0.78670 (12) | 0.0579 (5) |
| H2A | -0.0732 | 0.7000 | 0.7469 | 0.070* |
| C3 | 0.09943 (16) | 0.6248 (2) | 0.77016 (10) | 0.0508 (4) |
| C4 | 0.20312 (15) | 0.5587 (2) | 0.82741 (10) | 0.0432 (4) |
| C5 | 0.20019 (16) | 0.5199 (2) | 0.90521 (11) | 0.0493 (4) |
| H5A | 0.2696 | 0.4763 | 0.9460 | 0.059* |
| C6 | 0.09753 (18) | 0.5442 (3) | 0.92381 (12) | 0.0576 (5) |
| H6A | 0.0958 | 0.5161 | 0.9764 | 0.069* |
| C7 | 0.30928 (16) | 0.5142 (2) | 0.80365 (11) | 0.0487 (4) |
| C8 | 0.43130 (14) | 0.5720 (2) | 0.85556 (9) | 0.0392 (4) |
| C9 | 0.54611 (17) | 0.5086 (3) | 0.76135 (11) | 0.0550 (5) |
| H9A | 0.4968 | 0.5679 | 0.7142 | 0.066* |
| C10 | 0.68092 (17) | 0.3624 (3) | 0.84397 (12) | 0.0565 (5) |
| H10A | 0.7504 | 0.2943 | 0.8656 | 0.068* |
| C11 | 0.45564 (14) | 0.6885 (2) | 0.91621 (9) | 0.0393 (4) |
| H11A | 0.3900 | 0.7203 | 0.9317 | 0.047* |
| C12 | 0.56903 (15) | 0.7736 (2) | 0.96193 (9) | 0.0382 (4) |
| C13 | 0.65828 (16) | 0.8061 (2) | 0.92821 (10) | 0.0458 (4) |
| H13A | 0.6477 | 0.7676 | 0.8745 | 0.055* |
| C14 | 0.76122 (17) | 0.8936 (2) | 0.97250 (11) | 0.0528 (5) |
| H14A | 0.8206 | 0.9166 | 0.9494 | 0.063* |
| C15 | 0.77542 (17) | 0.9468 (2) | 1.05143 (12) | 0.0529 (5) |

| | | | | |
|------|--------------|------------|--------------|------------|
| C16 | 0.69124 (17) | 0.9189 (2) | 1.08757 (11) | 0.0509 (4) |
| H16A | 0.7039 | 0.9559 | 1.1419 | 0.061* |
| C17 | 0.58720 (16) | 0.8347 (2) | 1.04174 (10) | 0.0443 (4) |
| H17A | 0.5268 | 0.8179 | 1.0646 | 0.053* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| F1 | 0.0522 (7) | 0.1184 (11) | 0.1063 (10) | 0.0076 (7) | 0.0433 (7) | -0.0049 (9) |
| F2 | 0.0626 (8) | 0.1346 (12) | 0.0478 (6) | -0.0146 (7) | 0.0117 (5) | 0.0233 (7) |
| F3 | 0.0704 (8) | 0.0765 (8) | 0.0851 (9) | -0.0227 (7) | 0.0113 (7) | -0.0198 (7) |
| O1 | 0.0622 (9) | 0.1310 (14) | 0.0718 (9) | -0.0220 (9) | 0.0314 (8) | -0.0551 (10) |
| N1 | 0.0459 (8) | 0.0450 (8) | 0.0399 (7) | 0.0012 (7) | 0.0225 (6) | -0.0033 (6) |
| N2 | 0.0484 (9) | 0.0524 (9) | 0.0539 (9) | 0.0084 (7) | 0.0243 (7) | 0.0022 (7) |
| N3 | 0.0605 (11) | 0.0776 (12) | 0.0593 (10) | -0.0020 (9) | 0.0359 (9) | -0.0177 (9) |
| C1 | 0.0413 (11) | 0.0612 (12) | 0.0693 (13) | -0.0024 (9) | 0.0276 (9) | -0.0047 (10) |
| C2 | 0.0383 (10) | 0.0628 (12) | 0.0636 (12) | -0.0012 (9) | 0.0063 (9) | 0.0031 (10) |
| C3 | 0.0467 (11) | 0.0618 (11) | 0.0412 (9) | -0.0114 (9) | 0.0120 (8) | 0.0041 (9) |
| C4 | 0.0416 (10) | 0.0451 (9) | 0.0442 (9) | -0.0038 (8) | 0.0166 (8) | -0.0025 (8) |
| C5 | 0.0488 (10) | 0.0527 (11) | 0.0484 (10) | 0.0081 (9) | 0.0194 (8) | 0.0069 (8) |
| C6 | 0.0578 (12) | 0.0678 (13) | 0.0562 (11) | 0.0033 (10) | 0.0312 (10) | 0.0060 (10) |
| C7 | 0.0496 (10) | 0.0573 (11) | 0.0432 (9) | -0.0040 (9) | 0.0212 (8) | -0.0076 (9) |
| C8 | 0.0428 (9) | 0.0425 (9) | 0.0371 (8) | 0.0045 (7) | 0.0202 (7) | 0.0018 (7) |
| C9 | 0.0610 (12) | 0.0677 (12) | 0.0429 (10) | -0.0030 (10) | 0.0264 (9) | -0.0078 (9) |
| C10 | 0.0490 (11) | 0.0603 (12) | 0.0664 (12) | 0.0040 (9) | 0.0279 (10) | -0.0105 (10) |
| C11 | 0.0416 (9) | 0.0414 (9) | 0.0387 (8) | 0.0064 (7) | 0.0188 (7) | 0.0038 (7) |
| C12 | 0.0442 (9) | 0.0348 (8) | 0.0376 (8) | 0.0078 (7) | 0.0167 (7) | 0.0023 (7) |
| C13 | 0.0543 (11) | 0.0454 (10) | 0.0409 (9) | -0.0011 (9) | 0.0206 (8) | -0.0016 (8) |
| C14 | 0.0535 (11) | 0.0493 (11) | 0.0609 (11) | -0.0043 (9) | 0.0266 (9) | 0.0004 (9) |
| C15 | 0.0527 (11) | 0.0401 (10) | 0.0560 (11) | -0.0032 (9) | 0.0065 (9) | -0.0048 (9) |
| C16 | 0.0632 (12) | 0.0448 (10) | 0.0422 (9) | 0.0062 (9) | 0.0151 (9) | -0.0045 (8) |
| C17 | 0.0534 (11) | 0.0402 (9) | 0.0432 (9) | 0.0070 (8) | 0.0218 (8) | -0.0009 (8) |

Geometric parameters (Å, °)

| | | | |
|--------|-------------|----------|-----------|
| F1—C1 | 1.337 (2) | C5—H5A | 0.9300 |
| F2—C3 | 1.3382 (19) | C6—H6A | 0.9300 |
| F3—C15 | 1.341 (2) | C7—C8 | 1.465 (2) |
| O1—C7 | 1.199 (2) | C8—C11 | 1.323 (2) |
| N1—C9 | 1.323 (2) | C9—H9A | 0.9300 |
| N1—N2 | 1.351 (2) | C10—H10A | 0.9300 |
| N1—C8 | 1.414 (2) | C11—C12 | 1.443 (2) |
| N2—C10 | 1.298 (2) | C11—H11A | 0.9300 |
| N3—C9 | 1.300 (2) | C12—C13 | 1.383 (2) |
| N3—C10 | 1.336 (2) | C12—C17 | 1.385 (2) |
| C1—C6 | 1.345 (3) | C13—C14 | 1.359 (3) |
| C1—C2 | 1.355 (3) | C13—H13A | 0.9300 |
| C2—C3 | 1.357 (3) | C14—C15 | 1.361 (2) |

| | | | |
|--------------|--------------|----------------|--------------|
| C2—H2A | 0.9300 | C14—H14A | 0.9300 |
| C3—C4 | 1.365 (2) | C15—C16 | 1.352 (3) |
| C4—C5 | 1.373 (2) | C16—C17 | 1.362 (3) |
| C4—C7 | 1.479 (2) | C16—H16A | 0.9300 |
| C5—C6 | 1.362 (2) | C17—H17A | 0.9300 |
| C9—N1—N2 | 109.34 (14) | N1—C8—C7 | 113.87 (14) |
| C9—N1—C8 | 130.00 (15) | N3—C9—N1 | 110.95 (18) |
| N2—N1—C8 | 120.66 (12) | N3—C9—H9A | 124.5 |
| C10—N2—N1 | 101.56 (14) | N1—C9—H9A | 124.5 |
| C9—N3—C10 | 102.01 (15) | N2—C10—N3 | 116.13 (18) |
| F1—C1—C6 | 118.75 (17) | N2—C10—H10A | 121.9 |
| F1—C1—C2 | 117.86 (18) | N3—C10—H10A | 121.9 |
| C6—C1—C2 | 123.38 (17) | C8—C11—C12 | 129.55 (15) |
| C1—C2—C3 | 116.50 (18) | C8—C11—H11A | 115.2 |
| C1—C2—H2A | 121.7 | C12—C11—H11A | 115.2 |
| C3—C2—H2A | 121.7 | C13—C12—C17 | 117.96 (16) |
| F2—C3—C2 | 117.55 (17) | C13—C12—C11 | 123.14 (14) |
| F2—C3—C4 | 119.07 (16) | C17—C12—C11 | 118.80 (14) |
| C2—C3—C4 | 123.36 (16) | C14—C13—C12 | 120.92 (16) |
| C3—C4—C5 | 117.12 (16) | C14—C13—H13A | 119.5 |
| C3—C4—C7 | 121.05 (15) | C12—C13—H13A | 119.5 |
| C5—C4—C7 | 121.54 (16) | C13—C14—C15 | 118.50 (17) |
| C6—C5—C4 | 121.25 (17) | C13—C14—H14A | 120.8 |
| C6—C5—H5A | 119.4 | C15—C14—H14A | 120.8 |
| C4—C5—H5A | 119.4 | F3—C15—C16 | 118.53 (17) |
| C1—C6—C5 | 118.37 (17) | F3—C15—C14 | 118.29 (18) |
| C1—C6—H6A | 120.8 | C16—C15—C14 | 123.18 (17) |
| C5—C6—H6A | 120.8 | C15—C16—C17 | 117.69 (16) |
| O1—C7—C8 | 119.94 (16) | C15—C16—H16A | 121.2 |
| O1—C7—C4 | 119.85 (17) | C17—C16—H16A | 121.2 |
| C8—C7—C4 | 120.21 (15) | C16—C17—C12 | 121.70 (16) |
| C11—C8—N1 | 120.81 (15) | C16—C17—H17A | 119.2 |
| C11—C8—C7 | 125.23 (15) | C12—C17—H17A | 119.2 |
| C9—N1—N2—C10 | 0.01 (19) | O1—C7—C8—C11 | 166.70 (18) |
| C8—N1—N2—C10 | -179.18 (15) | C4—C7—C8—C11 | -12.5 (3) |
| F1—C1—C2—C3 | -179.89 (17) | O1—C7—C8—N1 | -9.9 (3) |
| C6—C1—C2—C3 | 1.0 (3) | C4—C7—C8—N1 | 170.88 (14) |
| C1—C2—C3—F2 | -179.47 (17) | C10—N3—C9—N1 | 0.6 (2) |
| C1—C2—C3—C4 | -1.0 (3) | N2—N1—C9—N3 | -0.4 (2) |
| F2—C3—C4—C5 | 178.52 (16) | C8—N1—C9—N3 | 178.68 (16) |
| C2—C3—C4—C5 | 0.1 (3) | N1—N2—C10—N3 | 0.4 (2) |
| F2—C3—C4—C7 | -7.6 (3) | C9—N3—C10—N2 | -0.6 (2) |
| C2—C3—C4—C7 | 173.93 (18) | N1—C8—C11—C12 | 7.1 (3) |
| C3—C4—C5—C6 | 0.9 (3) | C7—C8—C11—C12 | -169.35 (16) |
| C7—C4—C5—C6 | -172.91 (17) | C8—C11—C12—C13 | 29.3 (3) |
| F1—C1—C6—C5 | -179.18 (17) | C8—C11—C12—C17 | -154.43 (17) |

| | | | |
|--------------|--------------|-----------------|--------------|
| C2—C1—C6—C5 | -0.1 (3) | C17—C12—C13—C14 | 0.8 (2) |
| C4—C5—C6—C1 | -0.9 (3) | C11—C12—C13—C14 | 177.03 (16) |
| C3—C4—C7—O1 | -46.8 (3) | C12—C13—C14—C15 | 0.8 (3) |
| C5—C4—C7—O1 | 126.8 (2) | C13—C14—C15—F3 | 178.87 (16) |
| C3—C4—C7—C8 | 132.36 (19) | C13—C14—C15—C16 | -0.9 (3) |
| C5—C4—C7—C8 | -54.0 (2) | F3—C15—C16—C17 | 179.59 (15) |
| C9—N1—C8—C11 | -116.2 (2) | C14—C15—C16—C17 | -0.6 (3) |
| N2—N1—C8—C11 | 62.8 (2) | C15—C16—C17—C12 | 2.3 (3) |
| C9—N1—C8—C7 | 60.6 (2) | C13—C12—C17—C16 | -2.4 (2) |
| N2—N1—C8—C7 | -120.40 (17) | C11—C12—C17—C16 | -178.81 (15) |
