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2,2,2-Trifluoroethyl 5-methyl-1*H*-pyrazole-3-carboxylate

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AOB would like to dedicate this publication to his academic mentor on the occasion of his 70th birthday and to his contributions to solid-state chemistry, honoring the scientific tradition and the academic genealogical tree of Professor Dr Dr *h. c.* Joachim Strähle (University of Tübingen/Germany) and Professor Dr Hartmut Bärnighausen (University of Karlsruhe, now The Karlsruhe Institute of Technology/Germany).

Keywords: crystal structure; hydrogen-bonded chain; pyrazole.

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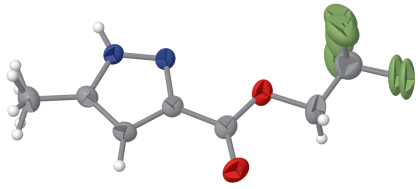
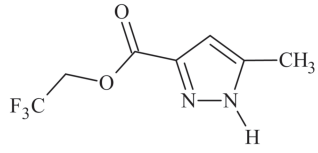
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_7H_7F_3N_2O_2$, which exhibits disorder over the terminal trifluoromethyl and methyl entities, is close to planar with the r.m.s. deviation for the non-H/-F atoms being 0.038 Å. In the crystal, the molecules are linked by N—H···N interactions into a [010] chain with a $C_1^1(3)$ motif. The Hirshfeld surface fingerprint plot analysis indicates that the major contributions for the crystal packing are from H···F/F···H (31.2%), H···H (15.9%), H···O/O···H (15.3%) and H···N/N···H (10.1%) contacts.

3D view



Chemical scheme



Structure description

As part of our interest in pyrazole derivatives with potential application in medicinal chemistry (Gonçalves *et al.*, 2016), we now report the crystal structure of the title compound, $C_7H_7F_3N_2O_2$ (**I**). For recent reports regarding pyrazole derivatives, see: Ameziane El Hassani *et al.* (2023), Ramajayam (2025) and Ríos & Portilla (2022).

There is one molecule in the asymmetric unit of (**I**), with all atoms being located in general positions (Fig. 1). The F atoms of the trifluoromethyl entity are disordered over two sets of sites in a 0.718 (11):0.282 (11) ratio and the H atoms of the C7 methyl group are statistically disordered. The molecule is close to planar, with the maximum deviations from the mean plane through the atoms being 0.0746 (17) Å for O1 [r.m.s.d. = 0.038 Å], excluding the hydrogen and the fluorine atoms. The side chain exhibits an extended conformation [C1*A*—C2—O1—C3 = −173.26 (19); C2—O1—C3—C4 = 178.48 (17)°].

In the crystal, the molecules are connected by N2—H2···N1 hydrogen bonds into a ribbon-like chain, which propagates along the *b*-axis direction (Table 1, Fig. 2). The crystal structure thus exhibits the supramolecular arrangement of a catemer with a $C_1^1(3)$ motif (Alkorta *et al.*, 2005; Foces-Foces *et al.*, 2000): the 'up' and 'down' catemers are related by centers of inversion and no strong or relevant interactions are observed between the supramolecular chains (Fig. 3). There are two short C—F···H contacts

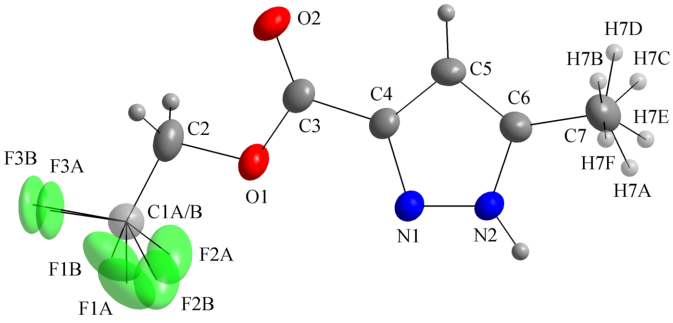


Figure 1
The molecular structure of (**I**) showing displacement ellipsoids drawn at the 40% probability level.

(Table 1), but their structure-directing significance is not clear due to the disordered F atoms. The Hirshfeld surface analysis analysis of (**I**) was performed with *Crystal Explorer 21* (Spackman *et al.*, 2021). The surface mapped over d_{norm} shows the regions with the strongest contacts in red in the vicinities of H2 and N1 (Fig. 4), being in agreement with previous figures (Figs. 2 and 3). The fingerprint plots (Fig. 5) indicate that the H···F/F···H (31.2%), H···H (15.9%), H···O/O···H (15.3%) and H ···N/N···H (10.1%) contacts are the most relevant for the crystal cohesion of (**I**).

A survey with the Cambridge Structural Database (CSD, accessed *via* WebCSD on January 2, 2026; Groom *et al.*, 2016) revealed a similar structure, namely ethyl-5-methyl-1*H*-pyrazole-3-carboxylate, $C_7H_{10}N_2O_2$ (CSD refcode: FAQSAR02; Kusakiewicz-Dawid *et al.*, 2019). The molecules of FAQSAR02 are linked by C—H···O and bifurcated N—H···(N,O) interactions into a two-dimensional tape-like supramolecular arrangement. Pyrazole derivatives show distinctive conformations in the solid state: it was pointed out by these authors that methyl and amino pyrazoles lead to structures with the amide or ester substituents and the N—H bond on the opposite side of the five-membered ring (compare C4 and N2 in this work, Fig. 1). This arrangement was observed in other structures, *e.g.* the derivatives with refcodes: HOKNON and HOKNUT. In contrast, nitro pyrazoles lead to

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N1^{i}	0.86	2.13	2.922 (2)	153
C7—H7A···F2A^{ii}	0.96	2.54	3.477 (7)	165
C7—H7D···F2B^{iii}	0.96	2.45	3.394 (11)	168

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{3}{2}, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

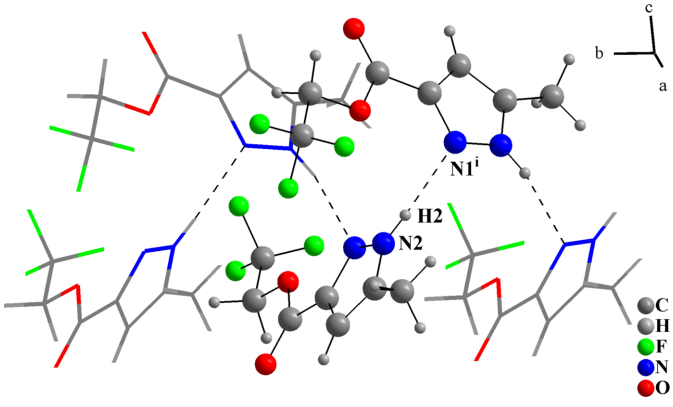


Figure 2
Fragment of the extended structure of (**I**) showing N—H···N hydrogen bonds. Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; minor disorder components omitted.

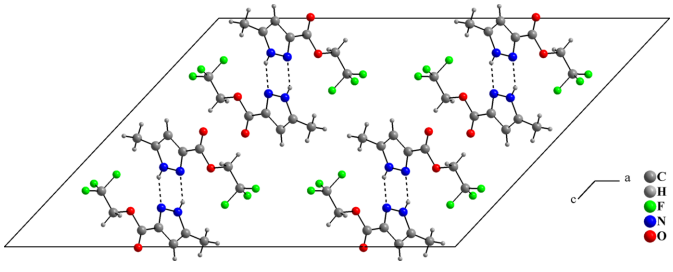


Figure 3
The packing of (**I**) as viewed along the *b*-axis direction.

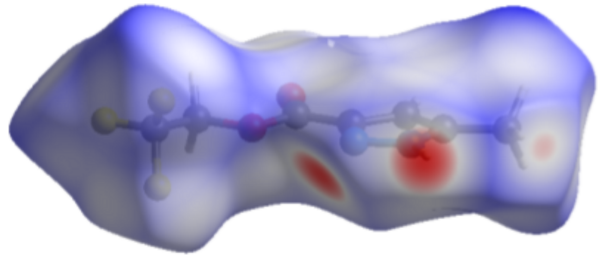


Figure 4
The Hirshfeld surface of (**I**) mapped over d_{norm} in the range −0.49 to 1.62 a. u.

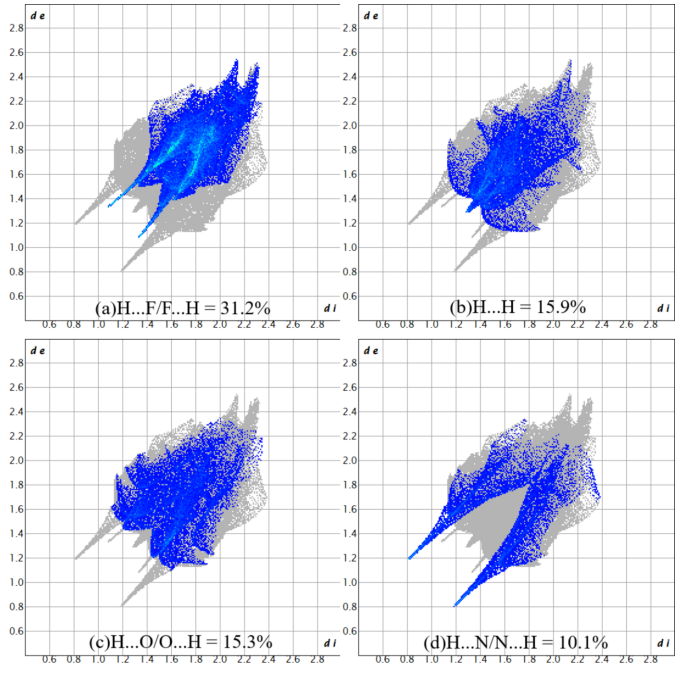


Figure 5
The two-dimensional fingerprint plots for (**I**) for different contact types.

the conformer with the N—H bond on the same side as the amide or carboxylate substituents, as observed in the structures with refcodes: HOKNED and HOKPIJ (Kusakiewicz-Dawid *et al.*, 2019).

Synthesis and crystallization

The synthesis and spectroscopic characterization of (**I**) are already published in the literature (Gonçalves *et al.*, 2016). For the single-crystal X-ray diffractometry reported here, colorless blocks of (**I**) were obtained from a dichloromethane solution by slow evaporation of the solvent at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The F atoms of the $-CF_3$ group are disordered over two sets of sites in a 0.718 (11) (*A* suffix) to 0.282 (11) (*B* suffix) ratio. The H atoms of the C7 methyl group are statistically disordered over two sets of sites.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_7F_3N_2O_2$
M_r	208.15
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	200
a, *b*, *c* (Å)	26.914 (6), 5.0133 (10), 18.693 (4)
β (°)	133.214 (2)
V (Å^3)	1838.2 (7)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.15
Crystal size (mm)	0.40 × 0.26 × 0.12
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.603, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10780, 2644, 1730
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.702
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.155, 1.04
No. of reflections	2644
No. of parameters	133
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.60

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 2006), *Crystal Explorer 21* (Spackman *et al.*, 2021) and *publCIF* (Westrip, 2010).

Acknowledgements

ABO is deeply grateful to his academic mentor, Prof Johannes Beck (University of Bonn), for the long-time support, *e.g.* the access to the X-ray diffractometer facility and fruitful discussions.

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full crystallographic data

IUCrData (2026). **11**, x260019 [https://doi.org/10.1107/S2414314626000192]

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2,2,2-Trifluoroethyl 5-methyl-1*H*-pyrazole-3-carboxylate

Crystal data

$C_7H_7F_3N_2O_2$
M_r = 208.15
Monoclinic, *C*2/*c*
a = 26.914 (6) Å
b = 5.0133 (10) Å
c = 18.693 (4) Å
β = 133.214 (2)°
V = 1838.2 (7) Å^3
Z = 8
F(000) = 848
D_x = 1.504 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3527 reflections
θ = 3.0–29.6°
μ = 0.15 mm^{-1}
T = 200 K
Prismatic, colourless
0.40 × 0.26 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: Fine-focus sealed tube
Horizontally mounted graphite crystal monochromator
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.603, T_{max} = 0.746
10780 measured reflections
2644 independent reflections
1730 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 29.9°, θ_{min} = 2.1°
h = −37→37
k = −4→7
l = −26→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.155
S = 1.04
2644 reflections
133 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
$w = 1/[\sigma^2(F_o^2) + (0.050P)^2 + 3.1537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C2	0.32947 (11)	1.0880 (5)	0.64954 (16)	0.0445 (5)	
H2A	0.309121	1.261903	0.637302	0.053*	
H2B	0.326834	1.046331	0.596343	0.053*	
C3	0.22953 (10)	0.8424 (4)	0.57173 (13)	0.0334 (4)	
C4	0.19776 (9)	0.6313 (4)	0.58381 (13)	0.0298 (4)	
C5	0.13094 (9)	0.5346 (4)	0.51236 (13)	0.0351 (5)	
H5	0.097239	0.590858	0.447569	0.042*	
C6	0.12582 (9)	0.3380 (4)	0.55871 (13)	0.0335 (4)	
C7	0.06852 (11)	0.1606 (5)	0.52476 (17)	0.0483 (6)	
H7A	0.085442	0.026166	0.573408	0.072*	0.5
H7B	0.048965	0.076990	0.464084	0.072*	0.5
H7C	0.034334	0.264684	0.514954	0.072*	0.5
H7D	0.027052	0.219061	0.461556	0.072*	0.5
H7E	0.063529	0.168237	0.570880	0.072*	0.5
H7F	0.078160	−0.019457	0.520010	0.072*	0.5
C1A	0.40082 (14)	1.0874 (6)	0.7439 (2)	0.0594 (7)*	0.718 (11)
F1A	0.4328 (3)	0.8643 (15)	0.7764 (6)	0.113 (2)	0.718 (11)
F2A	0.4018 (3)	1.1767 (14)	0.8164 (3)	0.0867 (16)	0.718 (11)
F3A	0.4367 (5)	1.253 (3)	0.7457 (9)	0.0838 (11)	0.718 (11)
C1B	0.40082 (14)	1.0874 (6)	0.7439 (2)	0.0594 (7)*	0.282 (11)
F1B	0.4233 (9)	0.839 (5)	0.7329 (14)	0.113 (2)	0.282 (11)
F2B	0.4209 (7)	1.060 (3)	0.8212 (8)	0.0867 (16)	0.282 (11)
F3B	0.4429 (15)	1.288 (8)	0.741 (2)	0.0838 (11)	0.282 (11)
N1	0.23275 (8)	0.5042 (4)	0.66983 (10)	0.0303 (4)	
N2	0.18769 (7)	0.3269 (3)	0.65185 (10)	0.0307 (4)	
H2	0.197260	0.217450	0.695247	0.037*	
O1	0.29450 (7)	0.8889 (3)	0.65623 (10)	0.0399 (4)	
O2	0.20159 (8)	0.9569 (3)	0.49600 (11)	0.0478 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0536 (12)	0.0447 (14)	0.0480 (12)	−0.0159 (11)	0.0397 (11)	−0.0078 (10)
C3	0.0428 (10)	0.0333 (12)	0.0332 (9)	−0.0012 (9)	0.0295 (8)	−0.0024 (8)
C4	0.0354 (9)	0.0313 (11)	0.0277 (8)	−0.0008 (8)	0.0236 (7)	−0.0017 (7)
C5	0.0330 (9)	0.0402 (13)	0.0251 (8)	0.0027 (9)	0.0172 (7)	0.0028 (8)
C6	0.0306 (9)	0.0360 (12)	0.0298 (8)	−0.0005 (8)	0.0191 (8)	−0.0012 (8)
C7	0.0359 (10)	0.0500 (15)	0.0482 (12)	−0.0071 (10)	0.0246 (10)	−0.0014 (11)
F1A	0.054 (2)	0.089 (2)	0.130 (5)	0.0057 (18)	0.038 (3)	0.018 (4)
F2A	0.088 (3)	0.121 (4)	0.0569 (11)	−0.051 (3)	0.0515 (16)	−0.045 (2)
F3A	0.070 (2)	0.095 (4)	0.0957 (18)	−0.0487 (18)	0.0607 (14)	−0.012 (2)
F1B	0.054 (2)	0.089 (2)	0.130 (5)	0.0057 (18)	0.038 (3)	0.018 (4)
F2B	0.088 (3)	0.121 (4)	0.0569 (11)	−0.051 (3)	0.0515 (16)	−0.045 (2)
F3B	0.070 (2)	0.095 (4)	0.0957 (18)	−0.0487 (18)	0.0607 (14)	−0.012 (2)
N1	0.0332 (7)	0.0330 (9)	0.0267 (7)	−0.0038 (7)	0.0213 (6)	−0.0016 (6)

N2	0.0326 (7)	0.0330 (10)	0.0263 (7)	−0.0019 (7)	0.0200 (6)	0.0028 (6)
O1	0.0445 (8)	0.0450 (10)	0.0343 (7)	−0.0127 (7)	0.0286 (6)	−0.0036 (6)
O2	0.0564 (9)	0.0490 (11)	0.0391 (8)	−0.0020 (8)	0.0331 (7)	0.0102 (7)

Geometric parameters (Å, º)

C2—O1	1.435 (2)	C7—H7A	0.9600
C2—C1A	1.470 (4)	C7—H7B	0.9600
C2—C1B	1.470 (4)	C7—H7C	0.9600
C2—H2A	0.9700	C7—H7D	0.9600
C2—H2B	0.9700	C7—H7E	0.9600
C3—O2	1.201 (2)	C7—H7F	0.9600
C3—O1	1.351 (2)	C1A—F3A	1.256 (7)
C3—C4	1.472 (3)	C1A—F1A	1.283 (8)
C4—N1	1.343 (2)	C1A—F2A	1.412 (6)
C4—C5	1.401 (3)	C1B—F2B	1.155 (11)
C5—C6	1.380 (3)	C1B—F1B	1.46 (3)
C5—H5	0.9300	C1B—F3B	1.539 (18)
C6—N2	1.355 (2)	N1—N2	1.347 (2)
C6—C7	1.494 (3)	N2—H2	0.8600
O1—C2—C1A	106.9 (2)	C6—C7—H7E	109.5
O1—C2—C1B	106.9 (2)	H7A—C7—H7E	56.3
O1—C2—H2A	110.3	H7B—C7—H7E	141.1
C1A—C2—H2A	110.3	H7C—C7—H7E	56.3
O1—C2—H2B	110.3	H7D—C7—H7E	109.5
C1A—C2—H2B	110.3	C6—C7—H7F	109.5
H2A—C2—H2B	108.6	H7A—C7—H7F	56.3
O2—C3—O1	124.09 (19)	H7B—C7—H7F	56.3
O2—C3—C4	124.35 (18)	H7C—C7—H7F	141.1
O1—C3—C4	111.56 (16)	H7D—C7—H7F	109.5
N1—C4—C5	111.54 (17)	H7E—C7—H7F	109.5
N1—C4—C3	121.32 (16)	F3A—C1A—F1A	108.1 (8)
C5—C4—C3	127.14 (17)	F3A—C1A—F2A	104.8 (7)
C6—C5—C4	105.27 (16)	F1A—C1A—F2A	104.8 (4)
C6—C5—H5	127.4	F3A—C1A—C2	112.3 (6)
C4—C5—H5	127.4	F1A—C1A—C2	118.2 (4)
N2—C6—C5	105.83 (17)	F2A—C1A—C2	107.5 (3)
N2—C6—C7	121.63 (19)	F2B—C1B—F1B	101.1 (9)
C5—C6—C7	132.54 (18)	F2B—C1B—C2	127.5 (7)
C6—C7—H7A	109.5	F1B—C1B—C2	99.2 (7)
C6—C7—H7B	109.5	F2B—C1B—F3B	113.0 (14)
H7A—C7—H7B	109.5	F1B—C1B—F3B	99.9 (19)
C6—C7—H7C	109.5	C2—C1B—F3B	110.3 (13)
H7A—C7—H7C	109.5	C4—N1—N2	103.93 (15)
H7B—C7—H7C	109.5	N1—N2—C6	113.44 (16)
C6—C7—H7D	109.5	N1—N2—H2	123.3
H7A—C7—H7D	141.1	C6—N2—H2	123.3

H7B—C7—H7D	56.3	C3—O1—C2	114.79 (16)
H7C—C7—H7D	56.3		
O2—C3—C4—N1	177.56 (19)	O1—C2—C1B—F1B	73.5 (9)
O1—C3—C4—N1	−1.6 (3)	O1—C2—C1B—F3B	177.7 (17)
O2—C3—C4—C5	−1.9 (3)	C5—C4—N1—N2	0.3 (2)
O1—C3—C4—C5	178.99 (18)	C3—C4—N1—N2	−179.26 (16)
N1—C4—C5—C6	0.0 (2)	C4—N1—N2—C6	−0.5 (2)
C3—C4—C5—C6	179.51 (19)	C5—C6—N2—N1	0.5 (2)
C4—C5—C6—N2	−0.3 (2)	C7—C6—N2—N1	−178.95 (18)
C4—C5—C6—C7	179.1 (2)	O2—C3—O1—C2	−0.6 (3)
O1—C2—C1A—F3A	179.1 (8)	C4—C3—O1—C2	178.48 (17)
O1—C2—C1A—F1A	52.1 (5)	C1A—C2—O1—C3	−173.26 (19)
O1—C2—C1A—F2A	−66.1 (4)	C1B—C2—O1—C3	−173.26 (19)
O1—C2—C1B—F2B	−38.3 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N1^{i}	0.86	2.13	2.922 (2)	153
C7—H7*A*···F2*A*^{ii}	0.96	2.54	3.477 (7)	165
C7—H7*D*···F2*B*^{iii}	0.96	2.45	3.394 (11)	168

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1/2, *y*−3/2, −*z*+3/2; (iii) *x*−1/2, −*y*+3/2, *z*−1/2.

Hydrogen-bond geometry (Å, °) and selected torsion angles (°) for the ethyl 5-methyl-1H-pyrazole-3-carboxylate derivative (Figs. 11 and 12; refcode: FAQSAR02; Kusakiewicz-Dawid et al., 2019)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*C*···O1^{i}	0.96	2.66	3.5453 (19)	153.9
N1—H1···N2^{ii}	0.86	2.17	2.9852 (18)	157.2
N1—H1···O2^{ii}	0.86	2.48	3.0998 (16)	129.3

Atom chains	**Torsion angles**	**Atom chains**	**Torsion angles**
C1/C2/C3/C4	179.66 (16)	C2/C1/C5/O1	-5.5 (3)
C1/C5/O2/C6	-179.37 (12)	C2/C1/C5/O2	173.72 (14)
C1/N2/N1/C3	-0.54 (16)	C5/O2/C6/C7	174.94 (12)

Symmetry codes: (i) -*x*+1/2, *y*+1/2, -*z*+1/2; (ii) -*x*+3/2, *y*+1/2, -*z*+1/2.