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Supporting information for article:

Crystal structures of the anhydrous and two solvated forms in methyl 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydro-pyrimidine-5-carboxylate

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S1. Computing details

For all structures, data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: SHELXT2014 (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

S2. 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (F1)

Table S1

Crystal data	
$C_{13}H_{13}FN_2O_3$	$F(000)$ = 1104
264.25	D_x = 1.382 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ Radiation, λ = 0.71073 Å
a = 16.0881 (15) Å	Cell parameters from 7891 reflections
b = 7.1958 (8) Å	θ = 2.7–29.9
c = 23.177 (3) Å	μ = 0.11 (mm^{-1})
β = 108.838 (4) °	T = 90 K
V = 2539.4 (5) Å^3	Plate, colourless
Z = 8	0.40 × 0.25 × 0.09 mm
Data collection	
Bruker *APEX*-II CCD diffractometer	3737 independent reflections
	2706 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.072
Absorption correction: Multi-scan (SADABS; Bruker, 2014)	θ_{max} = 30.1, θ_{min} = 2.7
	h = −22→22
T_{min} = 0.647, T_{max} = 0.746	k = −9→10
24306 measured reflections	l = −32→32
Refinement	
Refinement on F^2	Hydrogen site location: mixed
Least- squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 1.7817P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.115	
S = 1.02	
3737 reflections	$(\Delta/\sigma)_{max}$ = 0.001
182 parameters	$\Delta\rho_{max}$ = 0.39 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.26 e Å^{-3}

S2.1. Special Deatails

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.

Table S2 *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (A2)*

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.02856(6)	0.28689(14)	0.08155(5)	0.0212(2)
O2	-0.04829(6)	0.08374(13)	0.11713(4)	0.0183(2)
O3	0.19561(6)	-0.43566(13)	0.02354(4)	0.0159(2)
F1	0.42399(6)	0.14688(16)	0.28731(4)	0.0366(3)
N1	0.09065(7)	-0.34590(17)	0.06405(5)	0.0128(2)
H1A	0.07439(10)	-0.464(3)	0.0647(7)	0.020(4)
N2	0.17380(7)	-0.12694(16)	0.03515(5)	0.0126(2)
H2A	0.21529(11)	-0.100(2)	0.0197(8)	0.022(4)
C1	0.27321(9)	0.2129(2)	0.13482(6)	0.0173(3)
H1	0.263082	0.297493	0.101788	0.021*
C2	0.34316(9)	0.2433(2)	0.18837(7)	0.0229(3)
H2	0.381219	0.346839	0.192147	0.027*
C3	0.35521(9)	0.1195(2)	0.23523(6)	0.0233(3)
C4	0.30157(9)	-0.0309(2)	0.23263(6)	0.0231(3)
H4	0.311358	-0.112770	0.266334	0.028*
C5	0.23225(9)	-0.0593(2)	0.17878(6)	0.0190(3)
H5	0.193881	-0.161917	0.175722	0.023*
C6	0.21849(8)	0.06081(19)	0.12938(5)	0.0129(3)
C7	0.14667(8)	0.02117(18)	0.06901(5)	0.0112(2)
H7	0.136980	0.136887	0.043813	0.013*
C8	0.15738(8)	-0.30750(19)	0.04046(5)	0.0125(3)

C9	0.03494(8)	-0.21130(18)	0.07407(5)	0.0117(3)
C10	-0.04937(8)	-0.28875(19)	0.07810(6)	0.0140(3)
H10A	-0.039157	-0.343228	0.118554	0.021*
H10B	-0.071249	-0.384804	0.046890	0.021*
H10C	-0.092884	-0.188923	0.071487	0.021*
C11	0.06014(8)	-0.03197(19)	0.07743(5)	0.0115(3)
C12	0.01232(8)	0.12709(19)	0.09088(6)	0.0131(3)
C13	-0.09595(10)	0.2391(2)	0.13041(7)	0.0243(3)
H13A	-0.055451	0.318714	0.161158	0.036*
H13B	-0.141964	0.193158	0.145987	0.036*
H13C	-0.122776	0.310988	0.093100	0.036*

Table S3 *Atomic Displacement Parameters (Å²)*

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0216(5)	0.0117(5)	0.0346(6)	0.0019(4)	0.0152(4)	0.0002(4)
O2	0.0205(5)	0.0130(5)	0.0274(5)	0.0009(4)	0.0160(4)	0.0022(4)
O3	0.0169(4)	0.0130(5)	0.0209(5)	-0.0027(4)	0.0102(4)	0.0000(4)
F1	0.0219(4)	0.0623(7)	0.0188(4)	-0.0114(4)	-0.0030(3)	-0.0054(5)
N1	0.0142(5)	0.0089(6)	0.0089(6)	-0.0003(4)	0.0089(4)	-0.0015(4)
N2	0.0137(5)	0.0124(6)	0.0144(5)	-0.0021(4)	0.0085(4)	-0.0024(4)
C1	0.0168(6)	0.0183(7)	0.0182(6)	-0.0031(5)	0.0075(5)	-0.0034(5)
C2	0.0171(6)	0.0280(8)	0.0236(7)	-0.0096(6)	0.0066(5)	-0.0090(6)
C3	0.0142(6)	0.0389(10)	0.0151(6)	-0.0107(6)	0.0022(5)	-0.0009(6)
C4	0.0223(7)	0.0319(9)	0.0141(6)	0.0021(6)	0.0043(5)	0.0031(6)
C5	0.0186(6)	0.0212(8)	0.0168(6)	0.0003(6)	0.0054(5)	-0.0025(6)
C6	0.0115(5)	0.0154(7)	0.0128(5)	-0.0023(5)	0.0052(4)	0.0010(5)
C7	0.0119(5)	0.0094(6)	0.0131(5)	-0.0001(5)	0.0050(4)	-0.0002(5)
C8	0.0115(5)	0.0146(7)	0.0110(5)	-0.0014(5)	0.0033(4)	-0.0014(5)
C9	0.0111(5)	0.0141(7)	0.0103(5)	0.0012(5)	0.0041(4)	0.0004(5)

C10	0.0125(6)	0.0130(7)	0.0176(6)	0.0003(5)	0.0063(5)	-0.0016(5)
C11	0.0107(5)	0.0133(7)	0.0110(5)	0.0013(5)	0.0043(4)	0.0001(5)
C12	0.0115(5)	0.0139(7)	0.0139(5)	0.0005(5)	0.0041(4)	-0.0003(5)
C13	0.0252(7)	0.0190(8)	0.0362(8)	-0.0006(6)	0.0202(6)	0.0047(6)

Table S4 *Geometric parameters (Å, º)*

O1—C12	1.2140 (17)	C4—C5	1.3943 (18)
O2—C12	1.3422 (15)	C4—H4	0.9500
O2—C13	1.4441 (17)	C5—C6	1.3943 (19)
O3—C8	1.2403 (16)	C5—H5	0.9500
F1—C3	1.3630 (15)	C6—C7	1.5265 (16)
N1—C8	1.3809 (16)	C7—C11	1.5158 (17)
N1—C9	1.3890 (17)	C7—H7	1.0000
N1—H1A	0.891 (18)	C9—C11	1.3473 (19)
N2—C8	1.3395 (18)	C9—C10	1.4970 (17)
N2—C7	1.4709 (17)	C10—H10A	0.9800
N2—H2A	0.875 (17)	C10—H10B	0.9800
C1—C6	1.3845 (19)	C10—H10C	0.9800
C1—C2	1.3975 (19)	C11—C12	1.4676 (18)
C1—H1	0.9500	C13—H13A	0.9800
C2—C3	1.370 (2)	C13—H13B	0.9800
C2—H2	0.9500	C13—H13C	0.9800
C3—C4	1.373 (2)		
C12—O2—C13	115.48 (11)	N2—C7—H7	108.0
C8—N1—C9	123.55 (12)	C11—C7—H7	108.0

C8—N1—H1A	117.9 (10)	C6—C7—H7	108.0
C9—N1—H1A	117.0 (10)	O3—C8—N2	124.02 (11)
C8—N2—C7	123.53 (11)	O3—C8—N1	120.31 (12)
C8—N2—H2A	116.7 (11)	N2—C8—N1	115.60 (11)
C7—N2—H2A	117.2 (11)	C11—C9—N1	118.64 (11)
C6—C1—C2	120.71 (13)	C11—C9—C10	127.93 (12)
C6—C1—H1	119.6	N1—C9—C10	113.41 (11)
C2—C1—H1	119.6	C9—C10—H10A	109.5
C3—C2—C1	118.00 (14)	C9—C10—H10B	109.5
C3—C2—H2	121.0	H10A—C10—H10B	109.5
C1—C2—H2	121.0	C9—C10—H10C	109.5
F1—C3—C2	118.34 (14)	H10A—C10—H10C	109.5
F1—C3—C4	118.16 (14)	H10B—C10—H10C	109.5
C2—C3—C4	123.50 (13)	C9—C11—C12	126.21 (11)
C3—C4—C5	117.68 (13)	C9—C11—C7	120.39 (11)
C3—C4—H4	121.2	C12—C11—C7	113.38 (11)
C5—C4—H4	121.2	O1—C12—O2	122.04 (12)
C6—C5—C4	120.87 (13)	O1—C12—C11	122.90 (11)
C6—C5—H5	119.6	O2—C12—C11	114.99 (11)
C4—C5—H5	119.6	O2—C13—H13A	109.5
C1—C6—C5	119.20 (12)	O2—C13—H13B	109.5
C1—C6—C7	120.13 (11)	H13A—C13—H13B	109.5
C5—C6—C7	120.61 (12)	O2—C13—H13C	109.5
N2—C7—C11	109.21 (10)	H13A—C13—H13C	109.5

N2—C7—C6	110.93 (10)	H13B—C13—H13C	109.5
C11—C7—C6	112.58 (10)		
C6—C1—C2—C3	−0.6 (2)	C9—N1—C8—O3	−168.46 (11)
C1—C2—C3—F1	179.16 (12)	C9—N1—C8—N2	8.77 (17)
C1—C2—C3—C4	−1.0 (2)	C8—N1—C9—C11	−19.04 (18)
F1—C3—C4—C5	−179.00 (13)	C8—N1—C9—C10	159.33 (11)
C2—C3—C4—C5	1.1 (2)	N1—C9—C11—C12	−176.58 (11)
C3—C4—C5—C6	0.3 (2)	C10—C9—C11—C12	5.3 (2)
C2—C1—C6—C5	2.0 (2)	N1—C9—C11—C7	1.35 (17)
C2—C1—C6—C7	−175.37 (12)	C10—C9—C11—C7	−176.76 (11)
C4—C5—C6—C1	−1.8 (2)	N2—C7—C11—C9	21.92 (15)
C4—C5—C6—C7	175.52 (12)	C6—C7—C11—C9	−101.77 (13)
C8—N2—C7—C11	−33.69 (16)	N2—C7—C11—C12	−159.91 (10)
C8—N2—C7—C6	90.96 (14)	C6—C7—C11—C12	76.41 (13)
C1—C6—C7—N2	100.88 (14)	C13—O2—C12—O1	3.22 (18)
C5—C6—C7—N2	−76.42 (15)	C13—O2—C12—C11	−179.83 (11)
C1—C6—C7—C11	−136.40 (13)	C9—C11—C12—O1	−164.90 (13)
C5—C6—C7—C11	46.31 (16)	C7—C11—C12—O1	17.05 (17)
C7—N2—C8—O3	−163.16 (11)	C9—C11—C12—O2	18.17 (18)
C7—N2—C8—N1	19.72 (17)	C7—C11—C12—O2	−159.88 (10)

S3. 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (S1)

Table S5

Crystal data

$C_{53}H_{52}Cl_4F_4N_8O_{12}$	$F(000) = 1252$
$M_r = 1210.82$	$D_x = 1.508$ Mg m^{-3}
Monoclinic, $P2/n$	Mo $K\alpha$ Radiation, $\lambda = 0.71073$ Å
$a = 16.2070$ (7) Å	Cell parameters from 4823 reflections
$b = 9.1642$ (4) Å	$\theta = 2.5$–$28.6°$
$c = 17.9630$ (7) Å	$\mu = 0.31$ mm^{-1}
$\beta = 91.607$ (2)°	$T = 100$ K
$V = 2666.89$ (19) Å^3	Block, colourless
$Z = 2$	0.45 × 0.33 × 0.23 mm
Data collection	
Bruker *APEX*-II CCD Diffractometer	4601 independent reflections
	3571 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.051$
Absorption correction: Multi-scan (SADABS; Bruker, 2014)	$\theta_{max} = 25.0$, $\theta_{min} = 1.7$
	$h = -16 \rightarrow 19$
$T_{min} = 0.586$, $T_{max} = 0.746$	$k = -10 \rightarrow 10$
20706 measured reflections	$l = -19 \rightarrow 21$
Refinement	
Refinement on F^2	Hydrogen site location: mixed
Least- squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.067$	$w = 1/[\sigma^2(F_o^2) + (0.1858P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.242$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.56$ e Å^{-3}
4601 reflections	$\Delta\rho_{min} = -0.57$ e Å^{-3}
408 parameters	
22 restraints	

S3.1. Special Deatails

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.

Table S6

	x	*Y*	*Z*	U_{iso}*/U_{eq}
F1	0.94589(12)	0.7597(2)	0.67373(11)	0.0330(5)
F2	0.39469(13)	0.6525(2)	0.01540(11)	0.0379(6)

C27	1.2416(9)	0.9780(7)	0.2478(8)	0.041(2)
Cl1	1.17515(17)	0.9088(3)	0.31424(12)	0.0496(6)
Cl2	1.3229(6)	1.0678(8)	0.2941(4)	0.101(3)
Cl3	1.2793(2)	0.8335(3)	0.19447(15)	0.0682(8)
Cl4	1.1841(4)	1.0981(5)	0.1923(3)	0.0398(8)
O1	0.50525(14)	0.6145(2)	0.65445(12)	0.0231(6)
O2	0.57460(14)	0.4038(2)	0.64479(11)	0.0192(5)
O3	0.67518(13)	0.6295(2)	0.34185(11)	0.0176(5)
O4	0.75358(15)	1.2304(2)	0.09794(13)	0.0278(6)
O5	0.73355(13)	0.9987(2)	0.06299(11)	0.0186(5)
O6	0.56208(14)	0.9660(2)	0.36331(11)	0.0196(5)
N1	0.60477(16)	0.7117(3)	0.44123(13)	0.0136(6)
H1A	0.589(2)	0.779(4)	0.4184(19)	0.017(9)
N2	0.67468(16)	0.4950(3)	0.44849(13)	0.0144(6)
H2A	0.707(2)	0.431(4)	0.4249(17)	0.012(8)
N3	0.58642(17)	1.1304(3)	0.27159(14)	0.0158(6)
H3A	0.556(2)	1.190(4)	0.2983(18)	0.024(9)
N4	0.63691(15)	0.8970(2)	0.26442(13)	0.0130(6)
H4A	0.640(2)	0.813(2)	0.2853(16)	0.016
C1	0.7662(2)	0.5328(3)	0.64108(17)	0.0219(7)
H1	0.733166	0.465609	0.667369	0.026
C2	0.8326(2)	0.5994(4)	0.67717(17)	0.0235(8)
H2	0.845317	0.579132	0.728080	0.028
C3	0.87968(19)	0.6950(3)	0.63805(18)	0.0218(8)
C4	0.8638(2)	0.7285(3)	0.56485(17)	0.0193(7)
H4	0.897354	0.795600	0.539095	0.023
C5	0.79695(19)	0.6610(3)	0.52966(16)	0.0161(7)
H5	0.784825	0.682481	0.478782	0.019
C6	0.74721(18)	0.5632(3)	0.56640(15)	0.0139(7)

C7	0.67088(18)	0.4953(3)	0.52939(16)	0.0142(7)
H7	0.666652	0.391916	0.546685	0.017
C8	0.65441(19)	0.6121(3)	0.40688(16)	0.0142(7)
C9	0.56612(18)	0.6867(3)	0.50751(15)	0.0134(7)
C10	0.4952(2)	0.7857(3)	0.52126(17)	0.0192(7)
H10A	0.478142	0.833938	0.474629	0.029
H10B	0.511875	0.859532	0.558193	0.029
H10C	0.448992	0.728843	0.540007	0.029
C11	0.59344(18)	0.5765(3)	0.55241(15)	0.0129(6)
C12	0.55275(19)	0.5389(3)	0.62081(15)	0.0150(7)
C13	0.5341(2)	0.3521(3)	0.70969(17)	0.0231(7)
H13A	0.544531	0.247353	0.715802	0.035
H13B	0.474561	0.369020	0.703932	0.035
H13C	0.555542	0.404460	0.753688	0.035
C14	0.5803(2)	0.6954(3)	0.12916(15)	0.0172(7)
H14	0.622852	0.637081	0.151259	0.021
C15	0.5164(2)	0.6292(3)	0.08882(17)	0.0255(8)
H15	0.514218	0.526081	0.083460	0.031
C16	0.4565(2)	0.7160(3)	0.05699(17)	0.0224(8)
C17	0.4567(2)	0.8652(4)	0.06315(18)	0.0252(8)
H17	0.414351	0.922365	0.040080	0.030
C18	0.52112(19)	0.9305(3)	0.10436(17)	0.0188(7)
H18	0.522443	1.033603	0.109570	0.023
C19	0.58281(18)	0.8473(3)	0.13762(15)	0.0131(6)
C20	0.65285(19)	0.9133(3)	0.18480(15)	0.0135(6)
H20	0.704406	0.858123	0.174127	0.016
C21	0.59323(19)	0.9927(3)	0.30282(15)	0.0140(7)
C22	0.63275(18)	1.1757(3)	0.21263(15)	0.0141(7)
C23	0.6360(2)	1.3381(3)	0.20318(18)	0.0214(7)

H23A	0.683940	1.377053	0.231040	0.032
H23B	0.585455	1.381690	0.222062	0.032
H23C	0.640621	1.361774	0.150257	0.032
C24	0.66910(18)	1.0736(3)	0.16991(15)	0.0132(6)
C25	0.72154(18)	1.1124(3)	0.10920(16)	0.0155(7)
C26	0.7867(2)	1.0271(4)	0.00221(17)	0.0240(8)
H26A	0.791001	0.939168	-0.028515	0.036
H26B	0.841668	1.054326	0.021730	0.036
H26C	0.763902	1.107084	-0.028128	0.036

Table S7 *Atomic displacement parameters (Å^2)*

	U^{11}	U^{22}	U^{23}	U^{12}	U^{13}	U^{23}
F1	0.0209(11)	0.0409(12)	0.0364(11)	0.0012(9)	-0.0128(9)	-0.0103(9)
F2	0.0371(13)	0.0349(12)	0.0408(12)	-0.0064(9)	-0.0149(10)	-0.0214(10)
C27	0.050(6)	0.040(3)	0.033(3)	-0.002(8)	0.004(4)	0.002(7)
Cl1	0.0594(17)	0.0571(16)	0.0326(11)	0.0006(10)	0.0036(11)	-0.0251(12)
Cl2	0.090(5)	0.101(5)	0.110(5)	0.028(3)	-0.022(4)	-0.048(4)
Cl3	0.098(3)	0.0592(17)	0.0481(14)	-0.0001(13)	0.0050(15)	0.0329(17)
Cl4	0.0452(19)	0.0354(14)	0.0382(13)	-0.0167(12)	-0.0120(12)	0.0088(12)
O1	0.0282(14)	0.0178(12)	0.0235(12)	0.0002(9)	0.0035(10)	0.0040(10)
O2	0.0220(13)	0.0145(11)	0.0211(11)	0.0068(8)	0.0012(9)	0.0010(9)
O3	0.0251(13)	0.0126(11)	0.0152(11)	0.0002(8)	0.0020(9)	0.0043(9)
O4	0.0321(14)	0.0115(11)	0.0402(14)	0.0025(10)	0.0095(11)	-0.0077(10)
O5	0.0226(13)	0.0140(11)	0.0193(11)	0.0006(8)	0.0024(9)	-0.0048(9)
O6	0.0317(14)	0.0126(10)	0.0146(10)	0.0018(8)	0.0018(9)	0.0065(9)
N1	0.0201(15)	0.0073(12)	0.0136(12)	0.0033(10)	0.0004(10)	0.0047(10)
N2	0.0209(15)	0.0075(12)	0.0148(12)	-0.0012(9)	-0.0011(11)	0.0039(11)
N3	0.0195(15)	0.0086(12)	0.0190(13)	0.0001(10)	-0.0022(11)	0.0036(11)
N4	0.0165(14)	0.0061(12)	0.0162(12)	0.0035(9)	-0.0011(10)	0.0007(10)

C1	0.0213(18)	0.0234(17)	0.0208(15)	0.0066(13)	-0.0012(13)	0.0008(13)
C2	0.0212(18)	0.0301(18)	0.0190(15)	0.0055(13)	-0.0050(13)	-0.0014(14)
C3	0.0144(17)	0.0206(17)	0.0300(17)	-0.0019(13)	-0.0085(14)	-0.0003(13)
C4	0.0170(17)	0.0139(15)	0.0270(16)	0.0029(12)	0.0039(13)	0.0008(12)
C5	0.0186(17)	0.0129(15)	0.0168(15)	0.0033(11)	-0.0011(12)	0.0036(12)
C6	0.0140(16)	0.0104(14)	0.0172(14)	-0.0009(11)	-0.0019(12)	0.0075(12)
C7	0.0165(17)	0.0084(14)	0.0175(14)	0.0018(11)	-0.0015(12)	-0.0014(11)
C8	0.0179(16)	0.0075(14)	0.0167(15)	-0.0018(11)	-0.0051(12)	-0.0007(11)
C9	0.0153(16)	0.0101(14)	0.0148(14)	-0.0028(11)	-0.0021(12)	-0.0038(12)
C10	0.0237(18)	0.0148(15)	0.0193(15)	0.0013(12)	0.0007(13)	0.0064(13)
C11	0.0170(16)	0.0054(13)	0.0161(14)	-0.0003(11)	-0.0033(12)	-0.0014(11)
C12	0.0160(16)	0.0114(14)	0.0173(14)	0.0001(12)	-0.0045(12)	-0.0020(12)
C13	0.0263(19)	0.0213(17)	0.0215(16)	0.0084(13)	0.0004(14)	-0.0041(14)
C14	0.0239(18)	0.0119(15)	0.0159(14)	0.0016(11)	0.0004(13)	-0.0021(12)
C15	0.041(2)	0.0121(16)	0.0228(16)	-0.0021(12)	-0.0019(15)	-0.0098(14)
C16	0.0210(18)	0.0236(18)	0.0222(16)	-0.0047(13)	-0.0033(14)	-0.0118(14)
C17	0.0173(18)	0.0243(18)	0.0334(18)	0.0002(14)	-0.0103(14)	-0.0017(14)
C18	0.0170(17)	0.0110(15)	0.0283(16)	-0.0033(12)	-0.0034(13)	-0.0006(12)
C19	0.0164(16)	0.0094(14)	0.0136(14)	0.0000(11)	0.0030(11)	-0.0038(12)
C20	0.0146(16)	0.0085(14)	0.0171(14)	0.0017(11)	-0.0019(12)	0.0005(11)
C21	0.0181(16)	0.0086(14)	0.0147(14)	0.0007(11)	-0.0070(12)	-0.0001(12)
C22	0.0133(16)	0.0094(14)	0.0191(15)	0.0025(11)	-0.0070(12)	-0.0001(11)
C23	0.0253(19)	0.0071(15)	0.0315(17)	0.0021(12)	-0.0054(14)	0.0006(12)
C24	0.0129(15)	0.0080(14)	0.0184(14)	0.0022(11)	-0.0056(12)	-0.0030(11)
C25	0.0127(16)	0.0103(15)	0.0233(16)	0.0039(12)	-0.0040(12)	-0.0027(12)
C26	0.0252(19)	0.0261(18)	0.0210(16)	0.0033(13)	0.0015(13)	-0.0034(14)

Table S8 *Geometric parameters (Å, º)*

F1—C3	1.369 (3)	C5—H5	0.9500

F2—C16	1.364 (3)	C6—C7	1.521 (4)
C27—Cl4	1.738 (11)	C7—C11	1.526 (4)
C27—Cl2	1.744 (12)	C7—H7	1.0000
C27—Cl1	1.749 (12)	C9—C11	1.359 (4)
C27—Cl3	1.754 (10)	C9—C10	1.490 (4)
O1—C12	1.209 (4)	C10—H10A	0.9800
O2—C12	1.355 (3)	C10—H10B	0.9800
O2—C13	1.435 (4)	C10—H10C	0.9800
O3—C8	1.235 (4)	C11—C12	1.452 (4)
O4—C25	1.219 (4)	C13—H13A	0.9800
O5—C25	1.350 (4)	C13—H13B	0.9800
O5—C26	1.434 (4)	C13—H13C	0.9800
O6—C21	1.235 (4)	C14—C15	1.387 (4)
N1—C8	1.374 (4)	C14—C19	1.401 (4)
N1—C9	1.380 (4)	C14—H14	0.9500
N1—H1A	0.78 (3)	C15—C16	1.367 (5)
N2—C8	1.343 (4)	C15—H15	0.9500
N2—C7	1.456 (4)	C16—C17	1.372 (5)
N2—H2A	0.90 (4)	C17—C18	1.397 (4)
N3—C22	1.379 (4)	C17—H17	0.9500
N3—C21	1.385 (4)	C18—C19	1.380 (4)
N3—H3A	0.88 (4)	C18—H18	0.9500
N4—C21	1.332 (4)	C19—C20	1.523 (4)
N4—C20	1.468 (4)	C20—C24	1.517 (4)

N4—H4A	0.856 (18)	C20—H20	1.0000
C1—C2	1.383 (4)	C22—C24	1.355 (4)
C1—C6	1.396 (4)	C22—C23	1.499 (4)
C1—H1	0.9500	C23—H23A	0.9800
C2—C3	1.369 (5)	C23—H23B	0.9800
C2—H2	0.9500	C23—H23C	0.9800
C3—C4	1.368 (4)	C24—C25	1.446 (4)
C4—C5	1.384 (4)	C26—H26A	0.9800
C4—H4	0.9500	C26—H26B	0.9800
C5—C6	1.385 (4)	C26—H26C	0.9800
Cl4—C27—Cl2	111.1 (4)	C12—C11—C7	120.7 (2)
Cl4—C27—Cl1	106.9 (7)	O1—C12—O2	121.9 (3)
Cl2—C27—Cl1	108.5 (8)	O1—C12—C11	126.7 (3)
Cl4—C27—Cl3	110.7 (8)	O2—C12—C11	111.4 (3)
Cl2—C27—Cl3	110.3 (8)	O2—C13—H13A	109.5
Cl1—C27—Cl3	109.2 (4)	O2—C13—H13B	109.5
C12—O2—C13	116.0 (2)	H13A—C13—H13B	109.5
C25—O5—C26	115.4 (2)	O2—C13—H13C	109.5
C8—N1—C9	124.3 (3)	H13A—C13—H13C	109.5
C8—N1—H1A	118 (3)	H13B—C13—H13C	109.5
C9—N1—H1A	116 (3)	C15—C14—C19	120.7 (3)
C8—N2—C7	122.5 (2)	C15—C14—H14	119.7
C8—N2—H2A	113.2 (19)	C19—C14—H14	119.7
C7—N2—H2A	120.9 (19)	C16—C15—C14	118.3 (3)

C22—N3—C21	123.1 (3)	C16—C15—H15	120.8
C22—N3—H3A	123 (2)	C14—C15—H15	120.8
C21—N3—H3A	113 (2)	F2—C16—C15	118.9 (3)
C21—N4—C20	123.2 (2)	F2—C16—C17	118.0 (3)
C21—N4—H4A	113 (2)	C15—C16—C17	123.1 (3)
C20—N4—H4A	121 (2)	C16—C17—C18	118.0 (3)
C2—C1—C6	120.7 (3)	C16—C17—H17	121.0
C2—C1—H1	119.7	C18—C17—H17	121.0
C6—C1—H1	119.7	C19—C18—C17	120.9 (3)
C3—C2—C1	118.7 (3)	C19—C18—H18	119.5
C3—C2—H2	120.7	C17—C18—H18	119.5
C1—C2—H2	120.7	C18—C19—C14	118.9 (3)
C4—C3—C2	123.0 (3)	C18—C19—C20	122.8 (2)
C4—C3—F1	118.5 (3)	C14—C19—C20	118.3 (3)
C2—C3—F1	118.5 (3)	N4—C20—C24	107.9 (2)
C3—C4—C5	117.6 (3)	N4—C20—C19	110.7 (2)
C3—C4—H4	121.2	C24—C20—C19	114.6 (2)
C5—C4—H4	121.2	N4—C20—H20	107.8
C4—C5—C6	122.0 (3)	C24—C20—H20	107.8
C4—C5—H5	119.0	C19—C20—H20	107.8
C6—C5—H5	119.0	O6—C21—N4	124.2 (3)
C5—C6—C1	118.1 (3)	O6—C21—N3	120.4 (3)
C5—C6—C7	122.2 (2)	N4—C21—N3	115.3 (3)
C1—C6—C7	119.5 (3)	C24—C22—N3	118.8 (3)

N2—C7—C6	112.3 (2)	C24—C22—C23	127.2 (3)
N2—C7—C11	109.2 (2)	N3—C22—C23	114.0 (3)
C6—C7—C11	110.3 (2)	C22—C23—H23A	109.5
N2—C7—H7	108.3	C22—C23—H23B	109.5
C6—C7—H7	108.3	H23A—C23—H23B	109.5
C11—C7—H7	108.3	C22—C23—H23C	109.5
O3—C8—N2	124.1 (3)	H23A—C23—H23C	109.5
O3—C8—N1	121.2 (3)	H23B—C23—H23C	109.5
N2—C8—N1	114.7 (3)	C22—C24—C25	122.1 (3)
C11—C9—N1	119.1 (3)	C22—C24—C20	119.2 (3)
C11—C9—C10	126.5 (3)	C25—C24—C20	118.7 (3)
N1—C9—C10	114.4 (2)	O4—C25—O5	120.9 (3)
C9—C10—H10A	109.5	O4—C25—C24	127.3 (3)
C9—C10—H10B	109.5	O5—C25—C24	111.8 (2)
H10A—C10—H10B	109.5	O5—C26—H26A	109.5
C9—C10—H10C	109.5	O5—C26—H26B	109.5
H10A—C10—H10C	109.5	H26A—C26—H26B	109.5
H10B—C10—H10C	109.5	O5—C26—H26C	109.5
C9—C11—C12	122.0 (3)	H26A—C26—H26C	109.5
C9—C11—C7	117.3 (3)	H26B—C26—H26C	109.5
C6—C1—C2—C3	−0.4 (5)	C19—C14—C15—C16	0.7 (5)
C1—C2—C3—C4	0.4 (5)	C14—C15—C16—F2	178.1 (3)
C1—C2—C3—F1	−179.3 (3)	C14—C15—C16—C17	−0.1 (5)
C2—C3—C4—C5	−0.2 (5)	F2—C16—C17—C18	−178.6 (3)

F1—C3—C4—C5	179.5 (3)	C15—C16—C17—C18	−0.4 (5)
C3—C4—C5—C6	0.1 (4)	C16—C17—C18—C19	0.2 (5)
C4—C5—C6—C1	−0.2 (4)	C17—C18—C19—C14	0.3 (5)
C4—C5—C6—C7	176.4 (3)	C17—C18—C19—C20	−178.3 (3)
C2—C1—C6—C5	0.3 (5)	C15—C14—C19—C18	−0.8 (5)
C2—C1—C6—C7	−176.4 (3)	C15—C14—C19—C20	177.8 (3)
C8—N2—C7—C6	−82.3 (3)	C21—N4—C20—C24	39.2 (4)
C8—N2—C7—C11	40.4 (4)	C21—N4—C20—C19	−86.9 (3)
C5—C6—C7—N2	23.3 (4)	C18—C19—C20—N4	100.4 (3)
C1—C6—C7—N2	−160.1 (3)	C14—C19—C20—N4	−78.2 (3)
C5—C6—C7—C11	−98.9 (3)	C18—C19—C20—C24	−21.8 (4)
C1—C6—C7—C11	77.7 (3)	C14—C19—C20—C24	159.5 (3)
C7—N2—C8—O3	161.6 (3)	C20—N4—C21—O6	161.6 (3)
C7—N2—C8—N1	−21.0 (4)	C20—N4—C21—N3	−20.5 (4)
C9—N1—C8—O3	166.8 (3)	C22—N3—C21—O6	166.7 (3)
C9—N1—C8—N2	−10.7 (4)	C22—N3—C21—N4	−11.2 (4)
C8—N1—C9—C11	18.0 (4)	C21—N3—C22—C24	18.9 (4)
C8—N1—C9—C10	−160.6 (3)	C21—N3—C22—C23	−161.6 (3)
N1—C9—C11—C12	−176.5 (2)	N3—C22—C24—C25	−177.2 (2)
C10—C9—C11—C12	2.0 (4)	C23—C22—C24—C25	3.4 (4)
N1—C9—C11—C7	5.3 (4)	N3—C22—C24—C20	4.3 (4)
C10—C9—C11—C7	−176.2 (3)	C23—C22—C24—C20	−175.1 (3)
N2—C7—C11—C9	−30.9 (3)	N4—C20—C24—C22	−29.6 (3)
C6—C7—C11—C9	93.0 (3)	C19—C20—C24—C22	94.1 (3)

N2—C7—C11—C12	150.8 (2)	N4—C20—C24—C25	151.8 (2)
C6—C7—C11—C12	−85.2 (3)	C19—C20—C24—C25	−84.4 (3)
C13—O2—C12—O1	3.8 (4)	C26—O5—C25—O4	1.0 (4)
C13—O2—C12—C11	−176.4 (2)	C26—O5—C25—C24	−178.4 (2)
C9—C11—C12—O1	−17.8 (4)	C22—C24—C25—O4	16.5 (5)
C7—C11—C12—O1	160.3 (3)	C20—C24—C25—O4	−165.0 (3)
C9—C11—C12—O2	162.4 (2)	C22—C24—C25—O5	−164.0 (2)
C7—C11—C12—O2	−19.4 (3)	C20—C24—C25—O5	14.5 (3)

S4. 4-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (S2)

Table S9

Crystal data	
$C_{13}H_{13}FN_2O_3 \cdot 0.5(C_4H_8O_2)$	
M_r = 380.30	Z = 2
Triclinic, $P\bar{1}$	D_x = 1.400 Mg m^{-3}
a = 7.3353 (2) Å	Mo $K\alpha$ Radiation, λ = 0.71073 Å
b = 8.9091 (2) Å	Cell parameters from 3724 reflections
c = 12.5006 (4) Å	θ = 2.5–28.7°
α =82.389 (2)°	μ = 0.11 mm^{-1}
β = 79.380 (2)°	T = 100 K
γ = 65.898 (2)°	Rod, colourless
V = 731.44 (4) Å^3	0.43 × 0.36 × 0.27
Data collection	
Bruker *APEX*-II CCD diffractometer	3475 independent reflections
φ and ω scans	2647 reflections with $I > 2\sigma(I)$
Absorption correction: Multi-scan (SADABS; Bruker, 2014)	R_{int} = 0.034
T_{min} =0.706, T_{max} = 0.746	θ_{max} = 27.9, θ_{min} = 1.7
14325 measured reflections	h = −9→9
	k = −11→11
	l = −16→16
Refinement	
Refinement on F^2	Hydrogen site location: mixed
Least- squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.053	

$wR(F^2) = 0.141$	$1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.449P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3475 reflections	$(\Delta/\sigma)_{max} = 0.001$
398 parameters	$\Delta\rho_{max} = 0.65$ e Å^{-3}
118 restraints	$\Delta\rho_{min} = -0.34$ e Å^{-3}

S4.1. Special Deatails

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.

Table S10

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.71212(18)	-0.00939(16)	-0.00525(9)	0.0395(3)
O2	0.37279(18)	0.71184(14)	0.29141(11)	0.0255(3)
O1	0.25071(18)	0.52266(15)	0.36519(11)	0.0257(3)
O3	1.12712(17)	0.13882(14)	0.46283(10)	0.0221(3)
N1	0.9368(2)	0.38577(17)	0.38433(12)	0.0200(3)
H1A	1.033(4)	0.413(3)	0.3854(18)	0.033(6)
N2	0.8049(2)	0.18943(17)	0.44248(12)	0.0199(3)
H2A	0.828(3)	0.088(3)	0.4704(17)	0.029(5)
C1	0.7875(3)	0.2155(2)	0.18991(15)	0.0253(4)
H1	0.865664	0.276590	0.194367	0.030
C2	0.8095(3)	0.1448(2)	0.09401(16)	0.0283(4)
H2	0.901582	0.156310	0.032471	0.034
C3	0.6944(3)	0.0573(2)	0.09024(15)	0.0272(4)
C4	0.5615(3)	0.0362(2)	0.17711(16)	0.0299(4)
H4	0.485602	-0.026428	0.171991	0.036
C5	0.5402(3)	0.1084(2)	0.27287(15)	0.0245(4)
H5	0.447920	0.095876	0.333925	0.029
C6	0.6525(2)	0.19882(19)	0.28032(14)	0.0192(3)

C7	0.6294(2)	0.27781(19)	0.38548(14)	0.0177(3)
H7	0.507910	0.271437	0.434183	0.021
C8	0.9645(2)	0.2302(2)	0.43101(13)	0.0187(3)
C9	0.7506(2)	0.5048(2)	0.36381(14)	0.0196(4)
C10	0.7483(3)	0.6749(2)	0.34535(16)	0.0258(4)
H10A	0.804397	0.692116	0.269541	0.039
H10B	0.829798	0.688143	0.394445	0.039
H10C	0.609107	0.755813	0.359969	0.039
C11	0.5968(2)	0.45782(19)	0.36440(13)	0.0178(3)
C12	0.3918(2)	0.5651(2)	0.34235(14)	0.0197(3)
C13	0.1708(3)	0.8203(2)	0.27048(18)	0.0324(5)
H13A	0.126618	0.769881	0.220773	0.049
H13B	0.171257	0.926174	0.237192	0.049
H13C	0.078133	0.838225	0.339317	0.049
O4	1.0043(7)	0.3710(6)	-0.0909(4)	0.0739(11)
O5	1.0156(9)	0.5286(9)	0.0250(7)	0.0752(13)
C14	0.7037(14)	0.6047(12)	-0.0313(11)	0.101(2)
H14A	0.672799	0.670807	-0.099785	0.152
H14B	0.677212	0.677588	0.026965	0.152
H14C	0.618647	0.541383	-0.012401	0.152
C15	0.9215(17)	0.4887(15)	-0.0446(11)	0.0760(15)
C16	1.2183(13)	0.4257(11)	0.0214(9)	0.0803(15)
H16A	1.290889	0.431253	-0.053141	0.096
H16B	1.233320	0.310345	0.041144	0.096
C17	1.3007(11)	0.4794(8)	0.0976(7)	0.0792(17)
H17A	1.272184	0.596988	0.082200	0.119
H17B	1.447050	0.416554	0.090528	0.119
H17C	1.239131	0.461259	0.172016	0.119

Table S11 *Atomic displacement parameters (Å^2)*

	U^{11}	U^{22}	U^{23}	U^{12}	U^{13}	U^{23}
F1	0.0383(7)	0.0549(8)	0.0311(6)	-0.0157(6)	-0.0024(5)	-0.0213(6)
O2	0.0149(6)	0.0179(6)	0.0404(7)	0.0081(5)	-0.0059(5)	-0.0053(5)
O1	0.0163(6)	0.0201(6)	0.0419(8)	0.0032(5)	-0.0070(5)	-0.0090(5)
O3	0.0171(6)	0.0187(6)	0.0301(7)	0.0033(5)	-0.0079(5)	-0.0061(5)
N1	0.0145(7)	0.0171(7)	0.0302(8)	0.0026(6)	-0.0061(6)	-0.0081(6)
N2	0.0180(7)	0.0149(7)	0.0282(8)	0.0041(6)	-0.0085(6)	-0.0076(5)
C1	0.0214(9)	0.0241(9)	0.0320(10)	-0.0044(7)	-0.0004(7)	-0.0112(7)
C2	0.0231(9)	0.0304(9)	0.0292(10)	-0.0031(8)	0.0019(7)	-0.0104(8)
C3	0.0258(9)	0.0294(9)	0.0260(9)	-0.0072(7)	-0.0047(7)	-0.0084(8)
C4	0.0308(10)	0.0355(10)	0.0314(10)	-0.0036(8)	-0.0052(8)	-0.0206(8)
C5	0.0253(9)	0.0276(9)	0.0248(9)	0.0020(7)	-0.0043(7)	-0.0155(7)
C6	0.0162(8)	0.0149(7)	0.0253(8)	0.0014(6)	-0.0058(6)	-0.0046(6)
C7	0.0133(7)	0.0155(7)	0.0243(8)	0.0007(6)	-0.0042(6)	-0.0057(6)
C8	0.0170(8)	0.0171(7)	0.0216(8)	-0.0015(6)	-0.0027(6)	-0.0064(6)
C9	0.0165(8)	0.0155(7)	0.0257(9)	0.0010(6)	-0.0037(7)	-0.0053(6)
C10	0.0203(9)	0.0167(8)	0.0416(11)	0.0021(7)	-0.0081(8)	-0.0081(7)
C11	0.0150(8)	0.0145(7)	0.0228(8)	0.0003(6)	-0.0027(6)	-0.0051(6)
C12	0.0164(8)	0.0164(8)	0.0256(8)	-0.0005(6)	-0.0029(7)	-0.0061(6)
C13	0.0167(9)	0.0235(9)	0.0502(12)	0.0128(8)	-0.0078(8)	-0.0042(7)
O4	0.072(3)	0.063(2)	0.095(3)	-0.005(2)	-0.005(2)	-0.038(2)
O5	0.068(3)	0.042(2)	0.126(3)	-0.002(2)	-0.036(3)	-0.025(3)
C14	0.086(4)	0.059(4)	0.155(5)	-0.009(4)	-0.067(4)	-0.002(3)
C15	0.070(4)	0.044(2)	0.124(3)	0.000(2)	-0.032(3)	-0.027(3)
C16	0.071(3)	0.047(3)	0.128(4)	-0.002(3)	-0.038(3)	-0.019(3)
C17	0.074(4)	0.053(3)	0.109(4)	0.008(3)	-0.044(3)	-0.014(3)

Table S12 *Geometric parameters (Å, º)*

F1—C3	1.365 (2)	C7—H7	1.0000

O2—C12	1.340 (2)	C9—C11	1.352 (2)
O2—C13	1.451 (2)	C9—C10	1.496 (2)
O1—C12	1.216 (2)	C10—H10A	0.9800
O3—C8	1.2410 (19)	C10—H10B	0.9800
N1—C8	1.379 (2)	C10—H10C	0.9800
N1—C9	1.389 (2)	C11—C12	1.470 (2)
N1—H1A	0.84 (2)	C13—H13A	0.9800
N2—C8	1.340 (2)	C13—H13B	0.9800
N2—C7	1.465 (2)	C13—H13C	0.9800
N2—H2A	0.88 (2)	O4—C15	1.147 (14)
C1—C2	1.380 (3)	O5—C15	1.364 (9)
C1—C6	1.394 (2)	O5—C16	1.388 (10)
C1—H1	0.9500	C14—C15	1.499 (12)
C2—C3	1.373 (3)	C14—H14A	0.9800
C2—H2	0.9500	C14—H14B	0.9800
C3—C4	1.367 (3)	C14—H14C	0.9800
C4—C5	1.387 (3)	C16—C17	1.439 (12)
C4—H4	0.9500	C16—H16A	0.9900
C5—C6	1.387 (2)	C16—H16B	0.9900
C5—H5	0.9500	C17—H17A	0.9800
C6—C7	1.522 (2)	C17—H17B	0.9800
C7—C11	1.516 (2)	C17—H17C	0.9800
C12—O2—C13	115.75 (13)	H10A—C10—H10B	109.5
C8—N1—C9	123.70 (14)	C9—C10—H10C	109.5
C8—N1—H1A	114.2 (15)	H10A—C10—H10C	109.5
C9—N1—H1A	119.9 (15)	H10B—C10—H10C	109.5
C8—N2—C7	124.17 (14)	C9—C11—C12	126.50 (15)
C8—N2—H2A	114.0 (14)	C9—C11—C7	120.20 (14)
C7—N2—H2A	119.3 (14)	C12—C11—C7	113.27 (14)
C2—C1—C6	121.10 (17)	O1—C12—O2	122.16 (15)
C2—C1—H1	119.4	O1—C12—C11	122.79 (15)

C6—C1—H1	119.4	O2—C12—C11	115.01 (14)
C3—C2—C1	118.00 (17)	O2—C13—H13A	109.5
C3—C2—H2	121.0	O2—C13—H13B	109.5
C1—C2—H2	121.0	H13A—C13—H13B	109.5
F1—C3—C4	118.82 (17)	O2—C13—H13C	109.5
F1—C3—C2	118.19 (17)	H13A—C13—H13C	109.5
C4—C3—C2	122.99 (17)	H13B—C13—H13C	109.5
C3—C4—C5	118.44 (17)	C15—O5—C16	113.2 (6)
C3—C4—H4	120.8	C15—C14—H14A	109.5
C5—C4—H4	120.8	C15—C14—H14B	109.5
C6—C5—C4	120.63 (17)	H14A—C14—H14B	109.5
C6—C5—H5	119.7	C15—C14—H14C	109.5
C4—C5—H5	119.7	H14A—C14—H14C	109.5
C5—C6—C1	118.83 (16)	H14B—C14—H14C	109.5
C5—C6—C7	120.63 (15)	O4—C15—O5	120.3 (8)
C1—C6—C7	120.54 (15)	O4—C15—C14	130.7 (8)
N2—C7—C11	109.82 (13)	O5—C15—C14	108.3 (8)
N2—C7—C6	111.24 (13)	O5—C16—C17	108.1 (7)
C11—C7—C6	111.57 (13)	O5—C16—H16A	110.1
N2—C7—H7	108.0	C17—C16—H16A	110.1
C11—C7—H7	108.0	O5—C16—H16B	110.1
C6—C7—H7	108.0	C17—C16—H16B	110.1
O3—C8—N2	123.59 (15)	H16A—C16—H16B	108.4
O3—C8—N1	120.46 (15)	C16—C17—H17A	109.5
N2—C8—N1	115.90 (14)	C16—C17—H17B	109.5
C11—C9—N1	118.86 (14)	H17A—C17—H17B	109.5
C11—C9—C10	128.14 (15)	C16—C17—H17C	109.5
N1—C9—C10	112.99 (14)	H17A—C17—H17C	109.5
C9—C10—H10A	109.5	H17B—C17—H17C	109.5
C9—C10—H10B	109.5		
C6—C1—C2—C3	0.0 (3)	C8—N1—C9—C11	−16.4 (3)

C1—C2—C3—F1	178.43 (16)	C8—N1—C9—C10	162.49 (16)
C1—C2—C3—C4	−0.7 (3)	N1—C9—C11—C12	−178.65 (16)
F1—C3—C4—C5	−178.17 (16)	C10—C9—C11—C12	2.6 (3)
C2—C3—C4—C5	0.9 (3)	N1—C9—C11—C7	−0.9 (2)
C3—C4—C5—C6	−0.5 (3)	C10—C9—C11—C7	−179.65 (17)
C4—C5—C6—C1	−0.1 (3)	N2—C7—C11—C9	21.5 (2)
C4—C5—C6—C7	−179.88 (16)	C6—C7—C11—C9	−102.35 (18)
C2—C1—C6—C5	0.4 (3)	N2—C7—C11—C12	−160.51 (14)
C2—C1—C6—C7	−179.86 (16)	C6—C7—C11—C12	75.67 (18)
C8—N2—C7—C11	−30.2 (2)	C13—O2—C12—O1	3.2 (3)
C8—N2—C7—C6	93.77 (18)	C13—O2—C12—C11	−179.11 (16)
C5—C6—C7—N2	106.84 (17)	C9—C11—C12—O1	−164.82 (18)
C1—C6—C7—N2	−72.89 (19)	C7—C11—C12—O1	17.3 (2)
C5—C6—C7—C11	−130.15 (16)	C9—C11—C12—O2	17.5 (3)
C1—C6—C7—C11	50.1 (2)	C7—C11—C12—O2	−160.38 (14)
C7—N2—C8—O3	−166.08 (16)	C16—O5—C15—O4	7.2 (12)
C7—N2—C8—N1	16.3 (2)	C16—O5—C15—C14	178.5 (10)
C9—N1—C8—O3	−168.65 (16)	C15—O5—C16—C17	−180.0 (6)
C9—N1—C8—N2	9.1 (2)		