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1,1′,3,3′,5,5′-Hexamethylspiro[furo-[2,3-*d*]pyrimidine-6(5*H*),5′-pyrimidine]-2,2′,4,4′,6′(1*H*,3*H*,1′*H*,3′*H*,5′*H*)-pentaone

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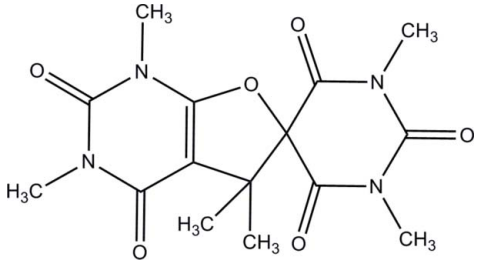
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.089; data-to-parameter ratio = 8.5.

In the title molecule, $C_{15}H_{18}N_4O_6$, the fused 2,3-dihydrofuran ring has an envelope conformation and the spiro pyrimidine ring has a half-chair conformation. In the crystal, short intermolecular O···C contacts of 2.835 (4) and 2.868 (4) Å between the carbonyl groups indicate the existence of electrostatic interactions, which link the molecules into corrugated sheets parallel to the *ab* plane.

Related literature

For applications of furo[2,3-*d*]pyrimidine derivatives, see Cody *et al.* (1997). For a related crystal structure, see Malathy Sony *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{18}N_4O_6$
M_r = 350.33
Orthorhombic, $P2_12_12_1$
a = 8.0122 (9) Å
b = 11.9181 (14) Å
c = 16.4037 (19) Å
V = 1566.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 120 K
0.21 × 0.14 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.980, T_{max} = 0.989
15042 measured reflections
1964 independent reflections
1589 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.089
S = 1.01
1964 reflections
232 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected interatomic distances (Å).

C8···O2^{i}	2.835 (4)	C3···O5^{ii}	2.868 (4)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: CV2553).

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supporting information

Acta Cryst. (2009). E**65**, o1444 [doi:10.1107/S1600536809019618]

1,1′,3,3′,5,5′-Hexamethylspiro[furo[2,3-*d*]pyrimidine-6(5*H*),5′-pyrimidine]-2,2′,4,4′,6′(1*H*,3*H*,1′*H*,3′*H*,5′*H*)-pentaone

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S1. Comment

Fused pyrimidine compounds are valued in view of their well-known biological properties. As example, the furo[2,3-*d*]pyrimidine antifolate derivative introduced as novel classical antitumor agent (Cody *et al.*, 1997). Herewith we present the title compound, (I).

In (I) (Fig. 1),the fused 2,3-dihydrofuran ring has an envelope conformation, and spiro pyrimidine ring has a half-chair conformation. Spiro pyrimidine ring is nearly perpendicular to 2,3-dihydro furan ring moiety, as was observed earlier in the related compound (Malathy Sony *et al.*, 2002). Torsion angles C2–C1–O4–C7 and C2–C1–C5–C6 are -99.39 (3)° and 94.87 (3)°, respectively. In the crystal, short intermolecular O···C contacts (Table 1) between the carbonyl groups prove an existing of electrostatic interactions, which link the molecules into corrugated sheets parallel to *ab* plane.

S2. Experimental

In a 50 ml round bottom flask (in an ice-bath) equipped with magnetic stirrer was added 200 mg (1.89 mmol) cyanogen bromide in 10 ml acetone. Then a solution of 295 mg (1.89 mmol) 1,3-dimethylbarbituric acid and 202 mg (2.00 mmol) triethylamine in acetone was added drop wise by reparatory funnel during 1 h. The white solid precipitated after few minutes and the color of liquid turned red. Initially, the precipitate was dissolved in acetone. A white crystalline colorless solid was formed after allowing the solution to stand overnight (228 mg, 50% yield) as a white crystalline solid, m.p. 210–212 °C (decomps.); FT—IR (KBr), *v*, cm^{-1}: 2981.54, 2954.71, 1689.08, 1646.35; ^{1}H NMR($CDCl_3$, 300 MHz) δ 3.434 (s, 3H); 3.355 (s, 6H), 3.283 (s, 3H), 1.402 (s,6*H*); ^{13}C NMR ($CDCl_3$, 75 MHz) δ 164.317, 160.207, 158.898, 151.033, 150.145, 93.220, 91.139, 53.872, 29.625, 29.081, 27.852, 23.318.

S3. Refinement

The C-bound H atoms were geometrically positioned (C–H 0.98 Å) and refined as riding, with U_{iso}(H) = 1.2-1.5 U_{eq}(C). In the absence of significant anomalous scatterers, 1855 Friedel pairs were merged before the final refinement.

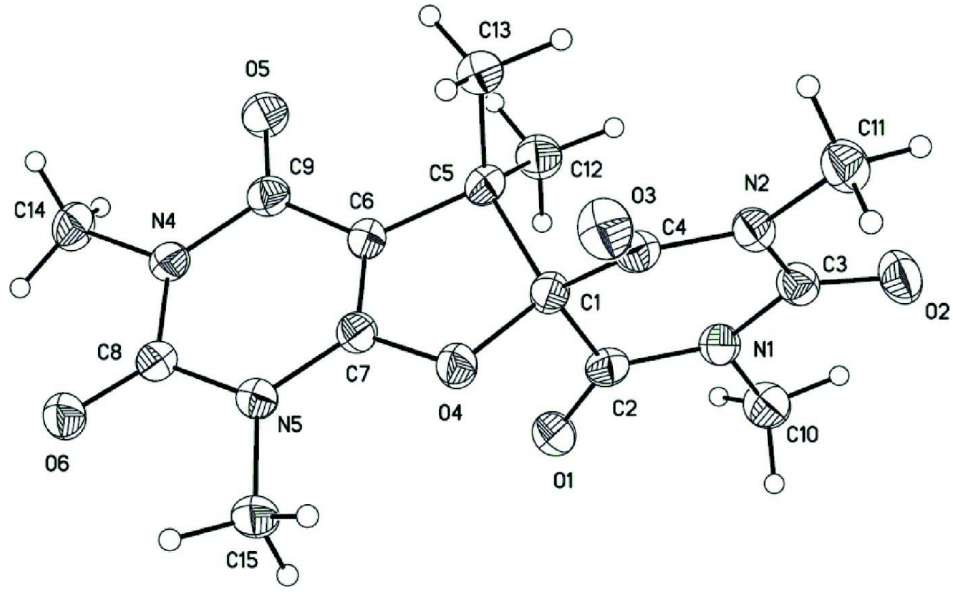

Figure 1

The molecular structure of the title compound showing the atomic numbering and 50% probability displacement ellipsoids.

1,1′,3,3′,5,5′-Hexamethylspiro[furo[2,3-*d*]pyrimidine-6(5*H*),5′- pyrimidine]-2,2′,4,4′,6′(1*H*,3*H*,1′*H*,3′*H*,5′*H*)-pentaone

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$c = 16.4037\ (19)$ Å
$V = 1566.4\ (3)$ Å^3
$Z = 4$
$F(000) = 736$
$D_x = 1.486$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 985 reflections
$\theta = 3$–25°
$\mu = 0.12$ mm^{-1}
$T = 120$ K
Prism, white
0.21 × 0.14 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.980$, $T_{max} = 0.989$
15042 measured reflections
1964 independent reflections
1589 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 27.0°$, $\theta_{min} = 2.1°$
$h = -10 \rightarrow 10$
$k = -15 \rightarrow 15$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.089$
$S = 1.01$
1964 reflections
232 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 2P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.20$ e Å^{-3}
	$\Delta\rho_{min} = -0.22$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5464 (3)	0.52840 (19)	0.75372 (15)	0.0307 (6)
O2	0.8328 (3)	0.8456 (2)	0.69785 (15)	0.0358 (6)
O3	0.6235 (3)	0.7991 (2)	0.94992 (14)	0.0352 (6)
O4	0.4987 (3)	0.59548 (19)	0.90811 (15)	0.0262 (5)
O5	−0.0582 (3)	0.6474 (2)	0.83863 (15)	0.0333 (6)
O6	0.0962 (3)	0.3545 (2)	1.00229 (15)	0.0306 (6)
N1	0.6700 (4)	0.6929 (2)	0.71936 (16)	0.0247 (6)
N2	0.6981 (4)	0.8365 (2)	0.81937 (16)	0.0251 (6)
N4	0.0212 (3)	0.5008 (2)	0.92003 (17)	0.0242 (6)
N5	0.3017 (3)	0.4687 (2)	0.95490 (17)	0.0242 (6)
C1	0.5068 (4)	0.6811 (3)	0.84600 (19)	0.0229 (7)
C2	0.5782 (4)	0.6254 (3)	0.7708 (2)	0.0250 (7)
C3	0.7394 (4)	0.7956 (3)	0.7427 (2)	0.0254 (7)
C4	0.6170 (4)	0.7750 (3)	0.8785 (2)	0.0252 (7)
C5	0.3186 (4)	0.7229 (3)	0.8311 (2)	0.0276 (8)
C6	0.2301 (4)	0.6208 (3)	0.8654 (2)	0.0242 (7)
C7	0.3382 (4)	0.5599 (3)	0.9086 (2)	0.0236 (7)
C8	0.1355 (4)	0.4355 (3)	0.9614 (2)	0.0237 (7)
C9	0.0562 (4)	0.5958 (3)	0.8712 (2)	0.0258 (8)
C10	0.7301 (5)	0.6431 (3)	0.6434 (2)	0.0334 (8)
H10A	0.6364	0.6084	0.6143	0.050*
H10B	0.8142	0.5858	0.6557	0.050*
H10C	0.7799	0.7016	0.6092	0.050*
C11	0.7816 (5)	0.9384 (3)	0.8465 (2)	0.0321 (8)
H11A	0.7027	0.9851	0.8771	0.048*
H11B	0.8223	0.9802	0.7990	0.048*
H11C	0.8760	0.9186	0.8817	0.048*
C12	0.2810 (5)	0.7474 (3)	0.7410 (2)	0.0337 (9)
H12A	0.1620	0.7645	0.7346	0.051*
H12B	0.3095	0.6817	0.7079	0.051*

H12C	0.3474	0.8119	0.7229	0.051*
C13	0.2770 (5)	0.8270 (3)	0.8822 (2)	0.0358 (9)
H13A	0.1572	0.8428	0.8784	0.054*
H13B	0.3400	0.8915	0.8615	0.054*
H13C	0.3072	0.8134	0.9392	0.054*
C14	−0.1530 (4)	0.4664 (3)	0.9244 (2)	0.0326 (8)
H14A	−0.1596	0.3889	0.9442	0.049*
H14B	−0.2034	0.4712	0.8701	0.049*
H14C	−0.2133	0.5159	0.9619	0.049*
C15	0.4309 (4)	0.3990 (3)	0.9914 (2)	0.0303 (8)
H15A	0.5206	0.4469	1.0123	0.045*
H15B	0.4760	0.3479	0.9501	0.045*
H15C	0.3830	0.3553	1.0363	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0313 (14)	0.0252 (12)	0.0355 (13)	−0.0023 (11)	0.0011 (12)	−0.0009 (11)
O2	0.0412 (15)	0.0304 (13)	0.0357 (14)	−0.0072 (13)	0.0071 (12)	0.0047 (11)
O3	0.0416 (16)	0.0377 (14)	0.0262 (12)	−0.0048 (13)	0.0006 (12)	−0.0017 (11)
O4	0.0207 (12)	0.0275 (12)	0.0304 (12)	−0.0015 (10)	−0.0002 (10)	0.0055 (11)
O5	0.0240 (12)	0.0359 (14)	0.0399 (14)	0.0027 (12)	−0.0043 (12)	0.0057 (12)
O6	0.0257 (13)	0.0307 (13)	0.0353 (13)	−0.0014 (11)	0.0014 (12)	0.0063 (12)
N1	0.0264 (15)	0.0257 (14)	0.0221 (13)	0.0007 (13)	0.0016 (12)	0.0010 (11)
N2	0.0262 (15)	0.0225 (14)	0.0267 (14)	−0.0013 (12)	0.0014 (13)	0.0002 (12)
N4	0.0215 (14)	0.0243 (14)	0.0269 (14)	0.0011 (12)	0.0009 (12)	−0.0002 (12)
N5	0.0228 (15)	0.0228 (14)	0.0268 (14)	0.0009 (12)	0.0004 (13)	0.0025 (12)
C1	0.0207 (15)	0.0247 (16)	0.0234 (16)	−0.0003 (14)	0.0014 (14)	0.0014 (14)
C2	0.0215 (16)	0.0264 (17)	0.0272 (17)	0.0033 (15)	−0.0023 (15)	0.0004 (15)
C3	0.0258 (18)	0.0242 (16)	0.0262 (16)	−0.0007 (15)	−0.0021 (15)	0.0017 (14)
C4	0.0227 (17)	0.0257 (17)	0.0274 (17)	0.0034 (14)	0.0007 (14)	0.0008 (14)
C5	0.0196 (16)	0.0285 (18)	0.0346 (18)	0.0030 (15)	0.0035 (15)	0.0044 (15)
C6	0.0218 (16)	0.0252 (17)	0.0255 (16)	0.0005 (14)	0.0028 (14)	0.0021 (14)
C7	0.0224 (17)	0.0210 (16)	0.0275 (17)	−0.0015 (15)	0.0016 (15)	−0.0016 (14)
C8	0.0225 (17)	0.0243 (17)	0.0244 (16)	0.0015 (15)	0.0015 (14)	−0.0005 (15)
C9	0.0267 (18)	0.0261 (18)	0.0248 (17)	0.0020 (15)	0.0005 (15)	−0.0016 (15)
C10	0.039 (2)	0.0317 (19)	0.0296 (18)	0.0008 (18)	0.0025 (17)	−0.0012 (16)
C11	0.0331 (19)	0.0269 (18)	0.0363 (19)	−0.0054 (16)	0.0001 (17)	−0.0015 (16)
C12	0.0284 (19)	0.0342 (19)	0.038 (2)	0.0031 (17)	−0.0037 (17)	0.0085 (17)
C13	0.0293 (19)	0.0268 (18)	0.051 (2)	0.0024 (16)	0.0097 (19)	0.0012 (18)
C14	0.0195 (17)	0.038 (2)	0.040 (2)	−0.0035 (17)	0.0002 (16)	0.0034 (17)
C15	0.0242 (17)	0.0302 (19)	0.0364 (19)	0.0043 (16)	−0.0023 (17)	0.0091 (16)

Geometric parameters (Å, º)

O1—C2	1.216 (4)	C5—C13	1.534 (5)
O2—C3	1.206 (4)	C5—C12	1.537 (5)
O3—C4	1.208 (4)	C6—C7	1.334 (5)

O4—C7	1.354 (4)	C6—C9	1.428 (5)
O4—C1	1.443 (4)	C10—H10A	0.9800
O5—C9	1.226 (4)	C10—H10B	0.9800
O6—C8	1.217 (4)	C10—H10C	0.9800
N1—C2	1.378 (4)	C11—H11A	0.9800
N1—C3	1.399 (4)	C11—H11B	0.9800
N1—C10	1.462 (4)	C11—H11C	0.9800
N2—C4	1.378 (4)	C12—H12A	0.9800
N2—C3	1.389 (4)	C12—H12B	0.9800
N2—C11	1.457 (4)	C12—H12C	0.9800
N4—C8	1.380 (4)	C13—H13A	0.9800
N4—C9	1.416 (4)	C13—H13B	0.9800
N4—C14	1.457 (4)	C13—H13C	0.9800
N5—C7	1.358 (4)	C14—H14A	0.9800
N5—C8	1.393 (4)	C14—H14B	0.9800
N5—C15	1.456 (4)	C14—H14C	0.9800
C1—C2	1.513 (4)	C15—H15A	0.9800
C1—C4	1.522 (5)	C15—H15B	0.9800
C1—C5	1.607 (5)	C15—H15C	0.9800
C5—C6	1.516 (5)		
C8···O2^{i}	2.835 (4)	C3···O5^{ii}	2.868 (4)
C7—O4—C1	105.6 (3)	O6—C8—N5	121.0 (3)
C2—N1—C3	123.8 (3)	N4—C8—N5	115.8 (3)
C2—N1—C10	117.4 (3)	O5—C9—N4	120.0 (3)
C3—N1—C10	117.2 (3)	O5—C9—C6	126.6 (3)
C4—N2—C3	124.3 (3)	N4—C9—C6	113.4 (3)
C4—N2—C11	116.4 (3)	N1—C10—H10A	109.5
C3—N2—C11	117.3 (3)	N1—C10—H10B	109.5
C8—N4—C9	126.8 (3)	H10A—C10—H10B	109.5
C8—N4—C14	116.9 (3)	N1—C10—H10C	109.5
C9—N4—C14	116.3 (3)	H10A—C10—H10C	109.5
C7—N5—C8	118.5 (3)	H10B—C10—H10C	109.5
C7—N5—C15	122.2 (3)	N2—C11—H11A	109.5
C8—N5—C15	119.1 (3)	N2—C11—H11B	109.5
O4—C1—C2	106.4 (3)	H11A—C11—H11B	109.5
O4—C1—C4	107.4 (3)	N2—C11—H11C	109.5
C2—C1—C4	112.9 (3)	H11A—C11—H11C	109.5
O4—C1—C5	106.5 (3)	H11B—C11—H11C	109.5
C2—C1—C5	111.5 (3)	C5—C12—H12A	109.5
C4—C1—C5	111.7 (3)	C5—C12—H12B	109.5
O1—C2—N1	121.7 (3)	H12A—C12—H12B	109.5
O1—C2—C1	121.7 (3)	C5—C12—H12C	109.5
N1—C2—C1	116.4 (3)	H12A—C12—H12C	109.5
O2—C3—N2	121.8 (3)	H12B—C12—H12C	109.5
O2—C3—N1	120.8 (3)	C5—C13—H13A	109.5
N2—C3—N1	117.3 (3)	C5—C13—H13B	109.5

O3—C4—N2	122.4 (3)	H13A—C13—H13B	109.5
O3—C4—C1	122.6 (3)	C5—C13—H13C	109.5
N2—C4—C1	114.7 (3)	H13A—C13—H13C	109.5
C6—C5—C13	110.2 (3)	H13B—C13—H13C	109.5
C6—C5—C12	114.7 (3)	N4—C14—H14A	109.5
C13—C5—C12	109.2 (3)	N4—C14—H14B	109.5
C6—C5—C1	97.7 (3)	H14A—C14—H14B	109.5
C13—C5—C1	111.8 (3)	N4—C14—H14C	109.5
C12—C5—C1	112.9 (3)	H14A—C14—H14C	109.5
C7—C6—C9	119.0 (3)	H14B—C14—H14C	109.5
C7—C6—C5	109.3 (3)	N5—C15—H15A	109.5
C9—C6—C5	130.4 (3)	N5—C15—H15B	109.5
C6—C7—O4	116.3 (3)	H15A—C15—H15B	109.5
C6—C7—N5	126.4 (3)	N5—C15—H15C	109.5
O4—C7—N5	117.3 (3)	H15A—C15—H15C	109.5
O6—C8—N4	123.1 (3)	H15B—C15—H15C	109.5

C7—O4—C1—C2	−99.4 (3)	C4—C1—C5—C13	−22.4 (4)
C7—O4—C1—C4	139.5 (3)	O4—C1—C5—C12	−141.8 (3)
C7—O4—C1—C5	19.7 (3)	C2—C1—C5—C12	−26.1 (4)
C3—N1—C2—O1	−166.1 (3)	C4—C1—C5—C12	101.2 (3)
C10—N1—C2—O1	−0.8 (5)	C13—C5—C6—C7	−101.6 (3)
C3—N1—C2—C1	19.0 (5)	C12—C5—C6—C7	134.8 (3)
C10—N1—C2—C1	−175.7 (3)	C1—C5—C6—C7	15.1 (4)
O4—C1—C2—O1	35.2 (4)	C13—C5—C6—C9	64.9 (5)
C4—C1—C2—O1	152.8 (3)	C12—C5—C6—C9	−58.7 (5)
C5—C1—C2—O1	−80.6 (4)	C1—C5—C6—C9	−178.4 (4)
O4—C1—C2—N1	−149.9 (3)	C9—C6—C7—O4	−172.6 (3)
C4—C1—C2—N1	−32.3 (4)	C5—C6—C7—O4	−4.3 (4)
C5—C1—C2—N1	94.4 (3)	C9—C6—C7—N5	4.8 (5)
C4—N2—C3—O2	−168.0 (3)	C5—C6—C7—N5	173.1 (3)
C11—N2—C3—O2	−4.5 (5)	C1—O4—C7—C6	−10.5 (4)
C4—N2—C3—N1	11.2 (5)	C1—O4—C7—N5	171.8 (3)
C11—N2—C3—N1	174.8 (3)	C8—N5—C7—C6	−2.2 (5)
C2—N1—C3—O2	172.2 (3)	C15—N5—C7—C6	171.9 (3)
C10—N1—C3—O2	6.9 (5)	C8—N5—C7—O4	175.2 (3)
C2—N1—C3—N2	−7.0 (5)	C15—N5—C7—O4	−10.7 (5)
C10—N1—C3—N2	−172.3 (3)	C9—N4—C8—O6	−179.9 (3)
C3—N2—C4—O3	158.8 (3)	C14—N4—C8—O6	−2.3 (5)
C11—N2—C4—O3	−4.9 (5)	C9—N4—C8—N5	1.2 (5)
C3—N2—C4—C1	−26.5 (5)	C14—N4—C8—N5	178.7 (3)
C11—N2—C4—C1	169.9 (3)	C7—N5—C8—O6	−179.8 (3)
O4—C1—C4—O3	−32.7 (4)	C15—N5—C8—O6	5.9 (5)
C2—C1—C4—O3	−149.7 (3)	C7—N5—C8—N4	−0.9 (5)
C5—C1—C4—O3	83.7 (4)	C15—N5—C8—N4	−175.1 (3)
O4—C1—C4—N2	152.5 (3)	C8—N4—C9—O5	−179.0 (3)
C2—C1—C4—N2	35.5 (4)	C14—N4—C9—O5	3.5 (5)
C5—C1—C4—N2	−91.1 (3)	C8—N4—C9—C6	1.3 (5)

O4—C1—C5—C6	−20.8 (3)	C14—N4—C9—C6	−176.3 (3)
C2—C1—C5—C6	94.9 (3)	C7—C6—C9—O5	176.2 (3)
C4—C1—C5—C6	−137.8 (3)	C5—C6—C9—O5	10.8 (6)
O4—C1—C5—C13	94.6 (3)	C7—C6—C9—N4	−4.1 (5)
C2—C1—C5—C13	−149.7 (3)	C5—C6—C9—N4	−169.5 (3)

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