Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-{[3-(4-Chlorophenyl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}-1,5-dimethyl-1*H*-1,5-benzodiazepine-2,4(3*H*,5*H*)-dione

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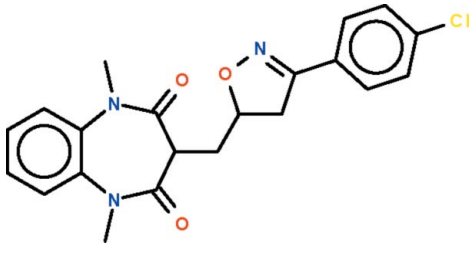
Received 20 February 2011; accepted 21 February 2011

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.066; wR factor = 0.184; data-to-parameter ratio = 17.1.

The seven-membered ring of the title molecule, $C_{21}H_{20}ClN_3O_3$, adopts a boat-shaped conformation (with the C atoms of the fused-ring as the stern and the methine C atom as the prow). The substituent at the 3-position occupies an equatorial position; its five-membered ring is approximately planar (r.m.s. deviation = 0.081 Å), and is aligned at 14.5 (1)° with respect to the chlorophenyl ring to which it is connected.

Related literature

For the crystal structure of the tetradecyl-substituted analog, see: Dardouri *et al.* (2011).



Experimental

Crystal data

$C_{21}H_{20}ClN_3O_3$
M_r = 397.85
Triclinic, $P\overline{1}$
a = 8.1821 (1) Å
b = 9.0741 (1) Å
c = 13.3792 (2) Å
α = 79.748 (1)°
β = 80.142 (1)°
γ = 85.910 (1)°
V = 962.19 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 295 K
0.40 × 0.30 × 0.20 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.915, T_{max} = 0.956
19243 measured reflections
4383 independent reflections
4056 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.184
S = 1.03
4383 reflections
256 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.83 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5479).

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supporting information

Acta Cryst. (2011). E**67**, o720 [doi:10.1107/S160053681100657X]

3-{[3-(4-Chlorophenyl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}-1,5-dimethyl-1*H*-1,5-benzodiazepine-2,4(3*H*,5*H*)-dione

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S1. Comment

The methylene part of 1,5-dimethyl-1,5-benzodiazepine-2,4-dione is relatively acidic, and one proton can be abstracted by using potassium *t*-butoxide; the resulting carbanion can undergo a nucleophlilic subsitution with a dibromoalkane to form 3-substituted derivatives. In a previous study, the compound was reacted with bromotetradecane to give the tetradecyl substitued derivative (Dardouri *et al.*, 2011). The title compound was obtained by using *p*-chlorobenzaldoxime to react with the ally group to furnish the title isoxazolinyl derivative (Scheme I, Fig. 1). The seven-membered ring of $C_{21}H_{20}ClN_3O_3$ adopts a boat-shaped conformation (with the C atoms of the fused-ring as the stern and the methine C atom as the prow). The substituent at the 3-position occupies an equatorial position.

S2. Experimental

To a solution of 3-allyl-1,5-dimethyl-1,5-benzodiazepine-2,4-dione (0.25 g, 1 mmol) and *p*-chlorobenzaldoxime (0.2 g, 1.3 mmol) in chloroform (10 ml) was added to a 4%solution of sodium hypochlorite solution (commerical bleach) (4 ml) at 273 K. Stirring was continued for 4 h. The organic layer was dried and the solvent evaporated under reduced pressure. The residue was then purified by column chromatography on silica gel by using a mixture of hexane and ethyl acetate (1/1) as eluent. Colorless crystals were isolated when the solvent was allowed to evaporate.

S3. Refinement

H-atoms were placed in calculated positions (C—H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C).

Omitted from the refinements were the following reflections because of being obscured by the beam stop and/or bad agreement between observed and calculated structure factors: (0 1 0), (1 1 0), (0 2 0), (2 3 0), (0 0 1), (1 1 1), (-1 1 2), (0 1 2) and (1 1 2).

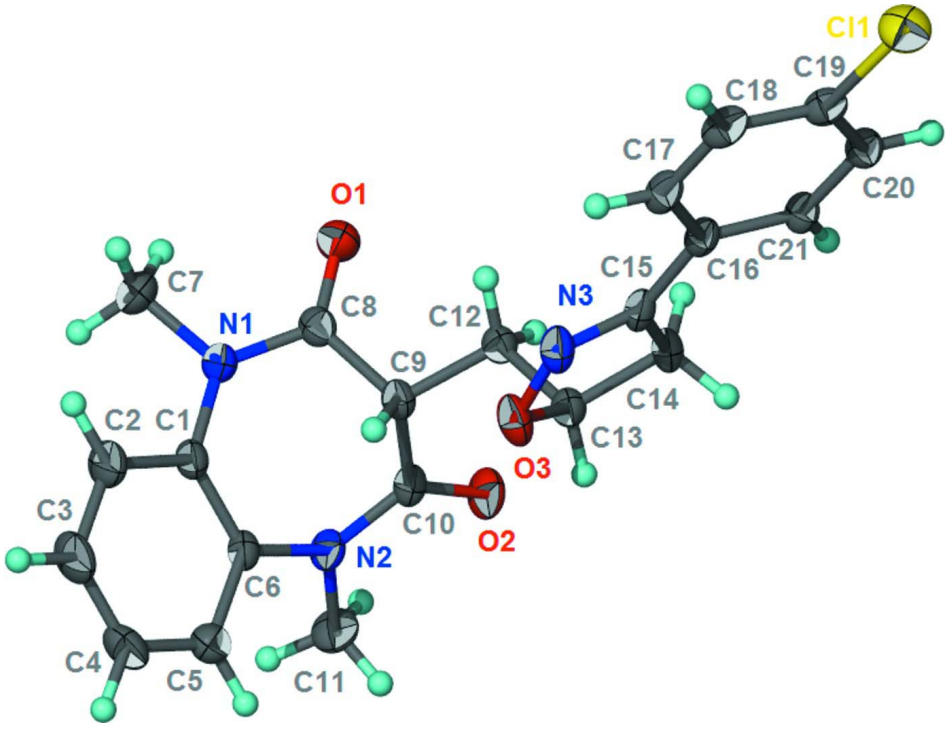

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{21}H_{20}ClN_3O_3$ at the 50% probability level; hydrogen atoms are drawn as arbitrary radius.

3-{[3-(4-Chlorophenyl)-4,5-dihydro-1,2-oxazol-5-yl]methyl}-1,5-dimethyl- 1*H*-1,5-benzodiazepine-2,4(3*H*,5*H*)-dione

Crystal data

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Hall symbol: -P 1
$a = 8.1821$ (1) Å
$b = 9.0741$ (1) Å
$c = 13.3792$ (2) Å
$\alpha = 79.748$ (1)°
$\beta = 80.142$ (1)°
$\gamma = 85.910$ (1)°
$V = 962.19$ (2) Å^3
$Z = 2$
$F(000) = 416$
$D_x = 1.373$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9887 reflections
$\theta = 3.0$–$30.7°$
$\mu = 0.23$ mm^{-1}
$T = 295$ K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker X8 APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.915$, $T_{max} = 0.956$
19243 measured reflections
4383 independent reflections
4056 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.184$
$S = 1.03$
4383 reflections
256 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
$w = 1/[\sigma^2(F_o^2) + (0.1062P)^2 + 0.889P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.83$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.046 (8)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.00333 (8)	0.14321 (7)	1.07254 (5)	0.0471 (2)
O1	0.2880 (2)	1.2329 (2)	0.66476 (13)	0.0428 (4)
O2	0.6469 (2)	1.2468 (2)	0.82002 (12)	0.0430 (4)
O3	0.6108 (2)	0.79540 (18)	0.76659 (12)	0.0400 (4)
N1	0.5122 (2)	1.2697 (2)	0.53908 (14)	0.0337 (4)
N2	0.7763 (2)	1.2907 (2)	0.65440 (13)	0.0310 (4)
N3	0.5112 (2)	0.6671 (2)	0.78978 (14)	0.0353 (4)
C1	0.6816 (3)	1.2379 (2)	0.50002 (15)	0.0309 (4)
C2	0.7216 (3)	1.2001 (3)	0.40171 (18)	0.0452 (6)
H2	0.6374	1.1910	0.3647	0.054*
C3	0.8856 (4)	1.1760 (4)	0.35894 (19)	0.0504 (7)
H3	0.9109	1.1522	0.2931	0.060*
C4	1.0116 (3)	1.1870 (3)	0.4132 (2)	0.0448 (6)
H4	1.1216	1.1710	0.3839	0.054*
C5	0.9744 (3)	1.2219 (3)	0.51136 (18)	0.0360 (5)
H5	1.0596	1.2275	0.5483	0.043*
C6	0.8100 (3)	1.2487 (2)	0.55536 (15)	0.0284 (4)
C7	0.4069 (3)	1.3563 (3)	0.46807 (19)	0.0449 (6)
H7A	0.3220	1.4127	0.5059	0.067*
H7B	0.3563	1.2889	0.4359	0.067*
H7C	0.4739	1.4237	0.4163	0.067*
C8	0.4365 (3)	1.2097 (2)	0.63486 (16)	0.0313 (4)
C9	0.5486 (3)	1.1145 (2)	0.70220 (15)	0.0293 (4)
H9	0.6178	1.0465	0.6616	0.035*
C10	0.6618 (3)	1.2213 (2)	0.73248 (15)	0.0301 (4)
C11	0.8826 (3)	1.3976 (3)	0.6799 (2)	0.0437 (6)
H11A	0.8160	1.4626	0.7216	0.065*
H11B	0.9365	1.4563	0.6177	0.065*
H11C	0.9648	1.3438	0.7173	0.065*
C12	0.4489 (3)	1.0212 (2)	0.79575 (16)	0.0307 (4)
H12A	0.4059	1.0846	0.8463	0.037*
H12B	0.3551	0.9814	0.7752	0.037*

C13	0.5550 (3)	0.8928 (2)	0.84372 (16)	0.0326 (4)
H13	0.6499	0.9304	0.8659	0.039*
C14	0.4547 (3)	0.7892 (2)	0.93283 (15)	0.0317 (4)
H14A	0.5181	0.7544	0.9881	0.038*
H14B	0.3515	0.8382	0.9599	0.038*
C15	0.4243 (3)	0.6634 (2)	0.87944 (15)	0.0301 (4)
C16	0.3142 (2)	0.5391 (2)	0.92464 (15)	0.0290 (4)
C17	0.2745 (3)	0.4381 (3)	0.86525 (16)	0.0352 (5)
H17	0.3144	0.4520	0.7950	0.042*
C18	0.1772 (3)	0.3186 (3)	0.90967 (18)	0.0367 (5)
H18	0.1508	0.2523	0.8698	0.044*
C19	0.1190 (3)	0.2982 (2)	1.01501 (17)	0.0330 (4)
C20	0.1526 (3)	0.3979 (2)	1.07529 (16)	0.0310 (4)
H20	0.1109	0.3840	1.1453	0.037*
C21	0.2496 (3)	0.5188 (2)	1.02965 (15)	0.0291 (4)
H21	0.2718	0.5871	1.0693	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0506 (4)	0.0392 (3)	0.0554 (4)	−0.0106 (2)	−0.0094 (3)	−0.0145 (3)
O1	0.0328 (8)	0.0558 (11)	0.0374 (9)	0.0037 (7)	−0.0019 (6)	−0.0071 (7)
O2	0.0561 (10)	0.0510 (10)	0.0238 (7)	−0.0044 (8)	−0.0058 (7)	−0.0114 (7)
O3	0.0490 (9)	0.0360 (8)	0.0274 (7)	0.0054 (7)	0.0083 (6)	−0.0011 (6)
N1	0.0331 (9)	0.0421 (10)	0.0258 (8)	−0.0033 (7)	−0.0058 (7)	−0.0037 (7)
N2	0.0381 (9)	0.0322 (9)	0.0248 (8)	−0.0041 (7)	−0.0079 (7)	−0.0063 (7)
N3	0.0432 (10)	0.0348 (9)	0.0241 (8)	0.0085 (8)	−0.0014 (7)	−0.0026 (7)
C1	0.0339 (10)	0.0360 (10)	0.0220 (9)	−0.0061 (8)	−0.0025 (7)	−0.0030 (7)
C2	0.0481 (13)	0.0640 (16)	0.0256 (10)	−0.0096 (11)	−0.0045 (9)	−0.0121 (10)
C3	0.0542 (15)	0.0698 (18)	0.0267 (11)	−0.0104 (13)	0.0074 (10)	−0.0166 (11)
C4	0.0384 (12)	0.0523 (14)	0.0400 (12)	−0.0074 (10)	0.0093 (10)	−0.0104 (11)
C5	0.0338 (11)	0.0379 (11)	0.0356 (11)	−0.0038 (8)	−0.0045 (8)	−0.0042 (9)
C6	0.0346 (10)	0.0284 (9)	0.0214 (9)	−0.0045 (7)	−0.0037 (7)	−0.0018 (7)
C7	0.0408 (12)	0.0581 (15)	0.0366 (12)	−0.0014 (11)	−0.0149 (10)	−0.0020 (11)
C8	0.0338 (10)	0.0339 (10)	0.0271 (10)	−0.0031 (8)	−0.0027 (8)	−0.0091 (8)
C9	0.0326 (10)	0.0301 (9)	0.0235 (9)	−0.0002 (7)	−0.0005 (7)	−0.0045 (7)
C10	0.0370 (10)	0.0306 (10)	0.0224 (9)	0.0026 (8)	−0.0059 (7)	−0.0042 (7)
C11	0.0472 (13)	0.0469 (13)	0.0433 (13)	−0.0099 (10)	−0.0154 (10)	−0.0137 (10)
C12	0.0292 (9)	0.0346 (10)	0.0267 (9)	−0.0003 (8)	−0.0023 (7)	−0.0030 (8)
C13	0.0309 (10)	0.0381 (11)	0.0263 (9)	0.0005 (8)	−0.0025 (7)	−0.0016 (8)
C14	0.0391 (11)	0.0322 (10)	0.0211 (9)	−0.0001 (8)	−0.0008 (8)	−0.0015 (7)
C15	0.0358 (10)	0.0327 (10)	0.0202 (8)	0.0085 (8)	−0.0057 (7)	−0.0033 (7)
C16	0.0311 (10)	0.0328 (10)	0.0237 (9)	0.0069 (8)	−0.0067 (7)	−0.0075 (7)
C17	0.0383 (11)	0.0450 (12)	0.0250 (9)	0.0090 (9)	−0.0086 (8)	−0.0145 (8)
C18	0.0383 (11)	0.0415 (12)	0.0374 (11)	0.0085 (9)	−0.0143 (9)	−0.0216 (9)
C19	0.0306 (10)	0.0337 (10)	0.0376 (11)	0.0033 (8)	−0.0095 (8)	−0.0116 (8)
C20	0.0337 (10)	0.0336 (10)	0.0267 (9)	0.0002 (8)	−0.0044 (8)	−0.0094 (8)
C21	0.0349 (10)	0.0304 (10)	0.0231 (9)	0.0029 (8)	−0.0056 (7)	−0.0085 (7)

Geometric parameters (Å, º)

Cl1—C19	1.738 (2)	C9—C12	1.523 (3)
O1—C8	1.228 (3)	C9—C10	1.536 (3)
O2—C10	1.218 (3)	C9—H9	0.9800
O3—N3	1.427 (3)	C11—H11A	0.9600
O3—C13	1.470 (3)	C11—H11B	0.9600
N1—C8	1.360 (3)	C11—H11C	0.9600
N1—C1	1.423 (3)	C12—C13	1.518 (3)
N1—C7	1.477 (3)	C12—H12A	0.9700
N2—C10	1.371 (3)	C12—H12B	0.9700
N2—C6	1.420 (3)	C13—C14	1.534 (3)
N2—C11	1.467 (3)	C13—H13	0.9800
N3—C15	1.282 (3)	C14—C15	1.506 (3)
C1—C2	1.397 (3)	C14—H14A	0.9700
C1—C6	1.403 (3)	C14—H14B	0.9700
C2—C3	1.384 (4)	C15—C16	1.471 (3)
C2—H2	0.9300	C16—C21	1.398 (3)
C3—C4	1.378 (4)	C16—C17	1.403 (3)
C3—H3	0.9300	C17—C18	1.376 (4)
C4—C5	1.383 (3)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.392 (3)
C5—C6	1.396 (3)	C18—H18	0.9300
C5—H5	0.9300	C19—C20	1.384 (3)
C7—H7A	0.9600	C20—C21	1.388 (3)
C7—H7B	0.9600	C20—H20	0.9300
C7—H7C	0.9600	C21—H21	0.9300
C8—C9	1.514 (3)		
N3—O3—C13	109.02 (15)	N2—C11—H11B	109.5
C8—N1—C1	123.46 (18)	H11A—C11—H11B	109.5
C8—N1—C7	117.58 (19)	N2—C11—H11C	109.5
C1—N1—C7	118.47 (18)	H11A—C11—H11C	109.5
C10—N2—C6	122.62 (17)	H11B—C11—H11C	109.5
C10—N2—C11	117.51 (18)	C13—C12—C9	111.22 (17)
C6—N2—C11	119.31 (18)	C13—C12—H12A	109.4
C15—N3—O3	109.03 (18)	C9—C12—H12A	109.4
C2—C1—C6	119.0 (2)	C13—C12—H12B	109.4
C2—C1—N1	118.8 (2)	C9—C12—H12B	109.4
C6—C1—N1	122.17 (18)	H12A—C12—H12B	108.0
C3—C2—C1	120.5 (2)	O3—C13—C12	107.78 (17)
C3—C2—H2	119.8	O3—C13—C14	103.57 (17)
C1—C2—H2	119.8	C12—C13—C14	112.48 (17)
C4—C3—C2	120.5 (2)	O3—C13—H13	110.9
C4—C3—H3	119.8	C12—C13—H13	110.9
C2—C3—H3	119.8	C14—C13—H13	110.9
C3—C4—C5	119.9 (2)	C15—C14—C13	100.88 (16)
C3—C4—H4	120.0	C15—C14—H14A	111.6

C5—C4—H4	120.0	C13—C14—H14A	111.6
C4—C5—C6	120.5 (2)	C15—C14—H14B	111.6
C4—C5—H5	119.7	C13—C14—H14B	111.6
C6—C5—H5	119.7	H14A—C14—H14B	109.4
C5—C6—C1	119.58 (19)	N3—C15—C16	120.6 (2)
C5—C6—N2	119.19 (19)	N3—C15—C14	114.1 (2)
C1—C6—N2	121.20 (18)	C16—C15—C14	125.22 (17)
N1—C7—H7A	109.5	C21—C16—C17	118.9 (2)
N1—C7—H7B	109.5	C21—C16—C15	119.55 (19)
H7A—C7—H7B	109.5	C17—C16—C15	121.59 (19)
N1—C7—H7C	109.5	C18—C17—C16	120.8 (2)
H7A—C7—H7C	109.5	C18—C17—H17	119.6
H7B—C7—H7C	109.5	C16—C17—H17	119.6
O1—C8—N1	122.1 (2)	C17—C18—C19	119.1 (2)
O1—C8—C9	122.53 (19)	C17—C18—H18	120.4
N1—C8—C9	115.32 (18)	C19—C18—H18	120.4
C8—C9—C12	111.58 (17)	C20—C19—C18	121.4 (2)
C8—C9—C10	107.09 (17)	C20—C19—Cl1	119.19 (17)
C12—C9—C10	112.23 (17)	C18—C19—Cl1	119.38 (17)
C8—C9—H9	108.6	C21—C20—C19	119.01 (19)
C12—C9—H9	108.6	C21—C20—H20	120.5
C10—C9—H9	108.6	C19—C20—H20	120.5
O2—C10—N2	122.0 (2)	C20—C21—C16	120.69 (19)
O2—C10—C9	121.92 (19)	C20—C21—H21	119.7
N2—C10—C9	116.09 (17)	C16—C21—H21	119.7
N2—C11—H11A	109.5		

C13—O3—N3—C15	−11.1 (2)	C11—N2—C10—C9	177.93 (19)
C8—N1—C1—C2	132.2 (2)	C8—C9—C10—O2	109.6 (2)
C7—N1—C1—C2	−39.5 (3)	C12—C9—C10—O2	−13.1 (3)
C8—N1—C1—C6	−50.2 (3)	C8—C9—C10—N2	−68.0 (2)
C7—N1—C1—C6	138.0 (2)	C12—C9—C10—N2	169.27 (17)
C6—C1—C2—C3	−1.0 (4)	C8—C9—C12—C13	162.03 (18)
N1—C1—C2—C3	176.6 (2)	C10—C9—C12—C13	−77.8 (2)
C1—C2—C3—C4	0.9 (4)	N3—O3—C13—C12	−101.45 (18)
C2—C3—C4—C5	0.2 (4)	N3—O3—C13—C14	17.9 (2)
C3—C4—C5—C6	−1.1 (4)	C9—C12—C13—O3	−61.8 (2)
C4—C5—C6—C1	1.0 (3)	C9—C12—C13—C14	−175.36 (17)
C4—C5—C6—N2	−177.2 (2)	O3—C13—C14—C15	−17.1 (2)
C2—C1—C6—C5	0.1 (3)	C12—C13—C14—C15	99.0 (2)
N1—C1—C6—C5	−177.46 (19)	O3—N3—C15—C16	−177.74 (17)
C2—C1—C6—N2	178.3 (2)	O3—N3—C15—C14	−1.2 (2)
N1—C1—C6—N2	0.7 (3)	C13—C14—C15—N3	12.0 (2)
C10—N2—C6—C5	−130.1 (2)	C13—C14—C15—C16	−171.60 (18)
C11—N2—C6—C5	41.1 (3)	N3—C15—C16—C21	165.85 (19)
C10—N2—C6—C1	51.7 (3)	C14—C15—C16—C21	−10.3 (3)
C11—N2—C6—C1	−137.1 (2)	N3—C15—C16—C17	−13.0 (3)
C1—N1—C8—O1	−176.2 (2)	C14—C15—C16—C17	170.9 (2)

C7—N1—C8—O1	−4.3 (3)	C21—C16—C17—C18	−1.7 (3)
C1—N1—C8—C9	4.7 (3)	C15—C16—C17—C18	177.11 (19)
C7—N1—C8—C9	176.56 (19)	C16—C17—C18—C19	−0.4 (3)
O1—C8—C9—C12	15.3 (3)	C17—C18—C19—C20	2.0 (3)
N1—C8—C9—C12	−165.63 (18)	C17—C18—C19—Cl1	−177.34 (16)
O1—C8—C9—C10	−107.9 (2)	C18—C19—C20—C21	−1.4 (3)
N1—C8—C9—C10	71.2 (2)	Cl1—C19—C20—C21	177.92 (15)
C6—N2—C10—O2	171.7 (2)	C19—C20—C21—C16	−0.8 (3)
C11—N2—C10—O2	0.3 (3)	C17—C16—C21—C20	2.3 (3)
C6—N2—C10—C9	−10.7 (3)	C15—C16—C21—C20	−176.55 (18)