Crystal structure of $C_{24}H_{32}N_2O_4$ — she0923

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Abstract

The crystal structure of $C_{24}H_{32}N_2O_4$ is reported.

Comment

The crystallographic asymmetric unit consists of one molecule of $C_{24}H_{32}N_2O_4$.

Experimental

The compound was prepared by MFS and was crystallized from dichloromethane/hexane. The sample ID is MFSA141-A3.

Refinement

H atoms were included at idealized positions (methyl groups aligned to best-match peaks in a difference electron density map) and were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98 Å) and with U_{iso}(H) in the range 1.2–1.5 times U_{eq} of the parent atom, after which they were refined with riding restraints. A difference map at this stage showed peaks between the H atoms attached to C18 and C27, suggesting rotational disorder of these methyl groups. The existing H sites were assigned occupancies of 0.7 and additional sites were generated between them with occupancies of 0.3.

The peaks in the final difference electron density map are located between C atoms.

Computing details

Data collection: *COLLECT* (Nonius, 1997-2001).; cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP*II (Johnson 1976) in *TEXSAN* (MSC, 1992-1997); software used to prepare material for publication: *CRYSTALS* (Betteridge *et al.*, 2003).

(she0923)

Crystal data

$C_{24}H_{32}N_2O_4$	$V = 4366.12\ (15)$ Å^3
$M_r = 412.53$	$Z = 8$
Orthorhombic, *Pbca*	Mo $K\alpha$
$a = 13.2821\ (3)$ Å	$\mu = 0.09$ mm^{-1}
$b = 10.5602\ (1)$ Å	$T = 200$ K
$c = 31.1284\ (7)$ Å	$0.50 \times 0.14 \times 0.07$ mm

Data collection

Area diffractometer	3853 independent reflections
Absorption correction: integration via Gaussian method (Coppens, 1970) implemented in maXus (2000)	2482 reflections with $I > 2.0\sigma(I)$
$T_{min} = 0.981$, $T_{max} = 0.995$	$R_{int} = 0.052$
38311 measured reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	271 parameters
$wR(F^2) = 0.156$	H-atom parameters constrained
$S = 0.89$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
3853 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °)

O17—C1	1.209 (2)	C6—C14	1.521 (2)
O19—C3	1.213 (2)	C7—C8	1.515 (3)
O26—C8	1.207 (2)	C7—C11	1.545 (2)
O28—C10	1.209 (3)	C10—C11	1.510 (3)
N2—C1	1.384 (3)	C11—C12	1.539 (3)
N2—C3	1.385 (2)	C12—C13	1.513 (3)
N2—C18	1.456 (2)	C13—C14	1.351 (2)
N9—C8	1.387 (3)	C13—C29	1.466 (3)
N9—C10	1.375 (3)	C14—C15	1.502 (2)
N9—C27	1.458 (3)	C15—C16	1.533 (2)
C1—C16	1.514 (3)	C20—C21	1.525 (2)
C3—C4	1.518 (2)	C21—C22	1.522 (3)
C4—C5	1.546 (2)	C22—C23	1.525 (3)
C4—C16	1.547 (2)	C23—C24	1.502 (3)
C5—C6	1.538 (2)	C24—C25	1.519 (3)
C5—C20	1.536 (2)	C29—C30	1.314 (3)
C6—C7	1.554 (2)		
C1—N2—C3	113.26 (15)	C7—C8—O26	128.12 (18)

C1—N2—C18	123.24 (17)	N9—C8—O26	123.30 (18)
C3—N2—C18	123.50 (17)	N9—C10—O28	124.61 (19)
C8—N9—C10	113.29 (16)	N9—C10—C11	108.79 (16)
C8—N9—C27	123.58 (19)	O28—C10—C11	126.6 (2)
C10—N9—C27	123.13 (19)	C7—C11—C10	104.88 (15)
N2—C1—O17	124.24 (19)	C7—C11—C12	113.53 (14)
N2—C1—C16	108.61 (15)	C10—C11—C12	109.23 (16)
O17—C1—C16	127.14 (18)	C11—C12—C13	111.12 (15)
N2—C3—O19	123.18 (17)	C12—C13—C14	115.99 (16)
N2—C3—C4	108.79 (15)	C12—C13—C29	120.82 (15)
O19—C3—C4	128.02 (18)	C14—C13—C29	123.18 (17)
C3—C4—C5	113.77 (14)	C6—C14—C13	117.84 (15)
C3—C4—C16	104.24 (14)	C6—C14—C15	115.70 (14)
C5—C4—C16	113.01 (14)	C13—C14—C15	126.43 (16)
C4—C5—C6	108.13 (14)	C14—C15—C16	110.11 (14)
C4—C5—C20	113.69 (14)	C4—C16—C15	113.44 (14)
C6—C5—C20	112.46 (14)	C4—C16—C1	104.91 (14)
C5—C6—C7	116.13 (14)	C15—C16—C1	109.20 (14)
C5—C6—C14	112.76 (14)	C5—C20—C21	114.81 (15)
C7—C6—C14	107.81 (13)	C20—C21—C22	112.54 (15)
C6—C7—C8	113.22 (14)	C21—C22—C23	114.66 (17)
C6—C7—C11	111.09 (14)	C22—C23—C24	114.80 (18)
C8—C7—C11	104.18 (14)	C23—C24—C25	112.1 (2)
C7—C8—N9	108.58 (16)	C13—C29—C30	127.1 (2)

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supplementary materials

Crystal structure of $C_{24}H_{32}N_2O_4$ — she0923

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(she0923)

Crystal data

$C_{24}H_{32}N_2O_4$	$D_x = 1.255$ Mg m^{-3}
$M_r = 412.53$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Orthorhombic, *Pbca*	Cell parameters from 36237 reflections
$a = 13.2821$ (3) Å	$\theta = 2.6$–25º
$b = 10.5602$ (1) Å	$\mu = 0.09$ mm^{-1}
$c = 31.1284$ (7) Å	$T = 200$ K
$V = 4366.12$ (15) Å^3	Needle, colourless
$Z = 8$	0.50 × 0.14 × 0.07 mm
$F_{000} = 1776$	

Data collection

Area diffractometer	2482 reflections with $I > 2.0\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 200$ K	$\theta_{max} = 25.0$º
φ & ω scans	$\theta_{min} = 2.6$º
Absorption correction: integration via Gaussian method (Coppens, 1970) implemented in maXus (2000)	$h = -15\rightarrow15$
$T_{min} = 0.981$, $T_{max} = 0.995$	$k = -12\rightarrow12$
38311 measured reflections	$l = -36\rightarrow36$
3853 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)] where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 59.9 94.4 47.1 11.8 0.00
$wR(F^2) = 0.156$	$(\Delta/\sigma)_{max} = 0.002$
$S = 0.89$	$\Delta\rho_{max} = 0.29$ e Å^{-3}
3853 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}

271 parameters
Primary atom site location: structure-invariant direct methods

Extinction correction: None

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O17	0.44487 (11)	0.67516 (15)	0.28247 (5)	0.0465	
O19	0.74753 (12)	0.87022 (13)	0.29778 (5)	0.0457	
O26	0.71864 (14)	0.54892 (14)	0.46344 (5)	0.0538	
O28	0.48857 (14)	0.79962 (19)	0.52937 (5)	0.0642	
N2	0.59032 (12)	0.79210 (15)	0.28390 (5)	0.0334	
N9	0.60299 (13)	0.65620 (16)	0.50378 (5)	0.0373	
C1	0.53119 (14)	0.68829 (18)	0.29392 (6)	0.0323	
C3	0.68579 (14)	0.78634 (17)	0.30166 (5)	0.0311	
C4	0.69725 (13)	0.66110 (16)	0.32512 (5)	0.0278	
C5	0.73412 (13)	0.67500 (17)	0.37200 (5)	0.0280	
C6	0.65544 (12)	0.75260 (15)	0.39690 (5)	0.0262	
C7	0.67457 (13)	0.76837 (17)	0.44585 (5)	0.0287	
C8	0.67113 (15)	0.64429 (18)	0.47026 (6)	0.0349	
C10	0.55291 (16)	0.7701 (2)	0.50380 (6)	0.0387	
C11	0.59144 (14)	0.84958 (17)	0.46696 (6)	0.0320	
C12	0.50356 (15)	0.88081 (18)	0.43654 (6)	0.0341	
C13	0.47317 (13)	0.76602 (17)	0.41050 (5)	0.0298	
C14	0.54892 (13)	0.70254 (15)	0.39109 (5)	0.0266	
C15	0.53943 (14)	0.58311 (17)	0.36520 (6)	0.0301	
C16	0.59210 (13)	0.59896 (16)	0.32171 (6)	0.0287	
C18	0.55500 (18)	0.8974 (2)	0.25774 (7)	0.0448	
C20	0.84057 (13)	0.73068 (18)	0.37586 (6)	0.0320	
C21	0.91976 (14)	0.66626 (18)	0.34793 (6)	0.0334	
C22	1.02537 (14)	0.71673 (19)	0.35617 (7)	0.0394	
C23	1.10758 (16)	0.6550 (2)	0.32913 (7)	0.0411	
C24	1.13613 (17)	0.5235 (2)	0.34282 (8)	0.0507	
C25	1.2190 (2)	0.4681 (3)	0.31493 (11)	0.0784	
C27	0.5851 (2)	0.5575 (2)	0.53562 (7)	0.0556	
C29	0.36745 (14)	0.72686 (18)	0.40778 (6)	0.0377	
C30	0.29290 (18)	0.7643 (3)	0.43247 (9)	0.0613	
H41	0.7458	0.6129	0.3088	0.0330*	
H51	0.7365	0.5881	0.3843	0.0321*	
H61	0.6580	0.8413	0.3851	0.0309*	
H71	0.7406	0.8061	0.4510	0.0329*	
H111	0.6192	0.9273	0.4790	0.0394*	
H121	0.4467	0.9132	0.4533	0.0407*	
H122	0.5250	0.9491	0.4173	0.0424*	
H151	0.5725	0.5117	0.3811	0.0358*	
H152	0.4688	0.5580	0.3606	0.0378*	
H161	0.5964	0.5182	0.3071	0.0342*	
H181	0.5706	0.9756	0.2699	0.0717*	0.7000
H182	0.4852	0.8915	0.2553	0.0725*	0.7000

H183	0.5844	0.8911	0.2299	0.0714*	0.7000
H184	0.5224	0.8656	0.2328	0.0720*	0.3000
H185	0.6108	0.9481	0.2495	0.0720*	0.3000
H186	0.5090	0.9472	0.2739	0.0720*	0.3000
H201	0.8609	0.7230	0.4059	0.0408*	
H202	0.8370	0.8199	0.3681	0.0404*	
H211	0.9183	0.5736	0.3536	0.0414*	
H212	0.9046	0.6797	0.3179	0.0404*	
H221	1.0406	0.7046	0.3866	0.0504*	
H222	1.0239	0.8097	0.3499	0.0500*	
H231	1.1698	0.7078	0.3299	0.0512*	
H232	1.0841	0.6501	0.2980	0.0510*	
H241	1.1593	0.5254	0.3727	0.0628*	
H242	1.0741	0.4699	0.3401	0.0627*	
H251	1.2361	0.3850	0.3242	0.1194*	
H252	1.2791	0.5233	0.3152	0.1183*	
H253	1.1964	0.4647	0.2850	0.1195*	
H271	0.5136	0.5560	0.5430	0.0870*	0.7000
H272	0.6268	0.5716	0.5602	0.0876*	0.7000
H273	0.6029	0.4784	0.5225	0.0854*	0.7000
H274	0.6468	0.5164	0.5422	0.0860*	0.3000
H275	0.5581	0.5943	0.5610	0.0860*	0.3000
H276	0.5387	0.4975	0.5244	0.0860*	0.3000
H291	0.3508	0.6680	0.3851	0.0470*	
H301	0.3055	0.8200	0.4555	0.0758*	
H302	0.2245	0.7344	0.4282	0.0739*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O17	0.0376 (8)	0.0543 (9)	0.0476 (9)	0.0002 (7)	−0.0119 (7)	−0.0017 (7)
O19	0.0512 (9)	0.0389 (8)	0.0470 (8)	−0.0125 (7)	−0.0041 (7)	0.0075 (6)
O26	0.0751 (11)	0.0393 (8)	0.0470 (8)	0.0185 (8)	−0.0009 (8)	0.0069 (7)
O28	0.0669 (11)	0.0866 (13)	0.0391 (8)	0.0105 (10)	0.0222 (8)	0.0075 (8)
N2	0.0402 (9)	0.0310 (8)	0.0288 (8)	0.0036 (6)	−0.0042 (6)	−0.0007 (6)
N9	0.0428 (9)	0.0404 (10)	0.0286 (8)	−0.0109 (7)	−0.0040 (7)	0.0070 (6)
C1	0.0346 (10)	0.0338 (9)	0.0285 (8)	0.0022 (7)	−0.0008 (7)	−0.0081 (7)
C3	0.0369 (10)	0.0299 (9)	0.0267 (8)	−0.0024 (8)	0.0024 (7)	−0.0057 (7)
C4	0.0283 (9)	0.0263 (9)	0.0288 (8)	0.0012 (7)	0.0024 (7)	−0.0052 (6)
C5	0.0293 (9)	0.0258 (8)	0.0288 (8)	0.0018 (7)	−0.0004 (7)	−0.0013 (7)
C6	0.0310 (9)	0.0226 (7)	0.0250 (8)	0.0009 (7)	0.0013 (7)	0.0002 (6)
C7	0.0293 (9)	0.0294 (9)	0.0273 (8)	−0.0021 (7)	−0.0001 (7)	−0.0038 (7)
C8	0.0406 (10)	0.0326 (9)	0.0316 (9)	−0.0016 (8)	−0.0096 (8)	0.0012 (7)
C10	0.0418 (11)	0.0471 (12)	0.0272 (9)	−0.0037 (9)	0.0013 (8)	0.0000 (8)
C11	0.0388 (10)	0.0293 (9)	0.0278 (9)	−0.0043 (7)	0.0030 (7)	−0.0058 (7)
C12	0.0395 (10)	0.0302 (9)	0.0325 (9)	0.0054 (8)	0.0046 (8)	−0.0029 (7)
C13	0.0319 (9)	0.0319 (9)	0.0256 (8)	0.0061 (7)	0.0008 (7)	0.0043 (7)
C14	0.0298 (9)	0.0255 (8)	0.0247 (8)	0.0010 (6)	−0.0001 (7)	0.0026 (7)

C15	0.0292 (8)	0.0266 (8)	0.0344 (9)	−0.0016 (7)	0.0006 (7)	−0.0003 (7)
C16	0.0301 (9)	0.0243 (9)	0.0317 (9)	0.0007 (7)	−0.0007 (7)	−0.0066 (7)
C18	0.0559 (13)	0.0397 (11)	0.0387 (10)	0.0109 (10)	−0.0049 (9)	0.0043 (8)
C20	0.0279 (9)	0.0351 (9)	0.0331 (9)	0.0008 (8)	−0.0002 (7)	−0.0062 (7)
C21	0.0306 (9)	0.0369 (9)	0.0327 (9)	0.0023 (8)	0.0009 (7)	−0.0034 (7)
C22	0.0319 (10)	0.0391 (11)	0.0473 (11)	−0.0010 (8)	0.0022 (8)	−0.0067 (9)
C23	0.0332 (10)	0.0418 (11)	0.0481 (12)	−0.0031 (8)	0.0090 (8)	0.0014 (9)
C24	0.0444 (11)	0.0520 (12)	0.0557 (13)	0.0109 (10)	0.0088 (11)	0.0103 (11)
C25	0.0626 (16)	0.0624 (17)	0.110 (2)	0.0248 (14)	0.0318 (17)	−0.0007 (17)
C27	0.0683 (15)	0.0593 (14)	0.0391 (11)	−0.0233 (12)	−0.0120 (11)	0.0210 (10)
C29	0.0328 (10)	0.0395 (10)	0.0407 (10)	0.0038 (8)	0.0022 (8)	0.0009 (8)
C30	0.0366 (11)	0.0764 (17)	0.0709 (16)	0.0014 (12)	0.0152 (11)	−0.0150 (14)

Geometric parameters (Å, °)

O17—C1	1.209 (2)	C16—H161	0.968
O19—C3	1.213 (2)	C18—H181	0.933
O26—C8	1.207 (2)	C18—H182	0.932
O28—C10	1.209 (3)	C18—H183	0.953
N2—C1	1.384 (3)	C18—H184	0.950
N2—C3	1.385 (2)	C18—H185	0.950
N2—C18	1.456 (2)	C18—H186	0.950
N9—C8	1.387 (3)	C20—C21	1.525 (2)
N9—C10	1.375 (3)	C20—H201	0.976
N9—C27	1.458 (3)	C20—H202	0.973
C1—C16	1.514 (3)	C21—C22	1.522 (3)
C3—C4	1.518 (2)	C21—H211	0.994
C4—C5	1.546 (2)	C21—H212	0.966
C4—C16	1.547 (2)	C22—C23	1.525 (3)
C4—H41	0.967	C22—H221	0.978
C5—C6	1.538 (2)	C22—H222	1.001
C5—C20	1.536 (2)	C23—C24	1.502 (3)
C5—H51	0.995	C23—H231	0.998
C6—C7	1.554 (2)	C23—H232	1.020
C6—C14	1.521 (2)	C24—C25	1.519 (3)
C6—H61	1.007	C24—H241	0.981
C7—C8	1.515 (3)	C24—H242	1.003
C7—C11	1.545 (2)	C25—H251	0.952
C7—H71	0.977	C25—H252	0.988
C10—C11	1.510 (3)	C25—H253	0.980
C11—C12	1.539 (3)	C27—H271	0.976
C11—H111	0.975	C27—H272	0.957
C12—C13	1.513 (3)	C27—H273	0.960
C12—H121	0.980	C27—H274	0.950
C12—H122	0.980	C27—H275	0.950
C13—C14	1.351 (2)	C27—H276	0.950
C13—C29	1.466 (3)	C29—C30	1.314 (3)
C14—C15	1.502 (2)	C29—H291	0.965
C15—C16	1.533 (2)	C30—H301	0.943

C15—H151	1.003	C30—H302	0.971
C15—H152	0.986		
O17···C18^{i}	3.189 (3)	N9···C30^{vi}	3.317 (3)
O19···C4^{ii}	3.271 (2)	N9···C27^{vii}	3.583 (3)
O19···C16^{ii}	3.306 (2)	C8···C30^{vi}	3.566 (3)
O26···C11^{iii}	3.287 (2)	C27···C27^{vii}	3.392 (5)
O26···C7^{iii}	3.330 (2)	C27···C30^{vi}	3.485 (4)
O28···C12^{iv}	3.539 (3)	C27···C29^{vii}	3.538 (3)
O28···C20^{v}	3.559 (2)		
C1—N2—C3	113.26 (15)	C4—C16—H161	110.6
C1—N2—C18	123.24 (17)	C15—C16—H161	110.2
C3—N2—C18	123.50 (17)	C1—C16—H161	108.2
C8—N9—C10	113.29 (16)	N2—C18—H181	112.2
C8—N9—C27	123.58 (19)	N2—C18—H182	108.4
C10—N9—C27	123.13 (19)	H181—C18—H182	108.3
N2—C1—O17	124.24 (19)	N2—C18—H183	108.9
N2—C1—C16	108.61 (15)	H181—C18—H183	109.9
O17—C1—C16	127.14 (18)	H182—C18—H183	109.1
N2—C3—O19	123.18 (17)	N2—C18—H184	109.5
N2—C3—C4	108.79 (15)	N2—C18—H185	109.3
O19—C3—C4	128.02 (18)	H184—C18—H185	109.5
C3—C4—C5	113.77 (14)	N2—C18—H186	109.6
C3—C4—C16	104.24 (14)	H184—C18—H186	109.5
C5—C4—C16	113.01 (14)	H185—C18—H186	109.5
C3—C4—H41	105.8	C5—C20—C21	114.81 (15)
C5—C4—H41	109.6	C5—C20—H201	107.3
C16—C4—H41	110.1	C21—C20—H201	108.5
C4—C5—C6	108.13 (14)	C5—C20—H202	107.8
C4—C5—C20	113.69 (14)	C21—C20—H202	108.9
C6—C5—C20	112.46 (14)	H201—C20—H202	109.4
C4—C5—H51	106.6	C20—C21—C22	112.54 (15)
C6—C5—H51	108.6	C20—C21—H211	108.9
C20—C5—H51	107.1	C22—C21—H211	109.4
C5—C6—C7	116.13 (14)	C20—C21—H212	110.0
C5—C6—C14	112.76 (14)	C22—C21—H212	107.7
C7—C6—C14	107.81 (13)	H211—C21—H212	108.2
C5—C6—H61	106.8	C21—C22—C23	114.66 (17)
C7—C6—H61	104.7	C21—C22—H221	107.9
C14—C6—H61	108.2	C23—C22—H221	109.3
C6—C7—C8	113.22 (14)	C21—C22—H222	107.0
C6—C7—C11	111.09 (14)	C23—C22—H222	109.0
C8—C7—C11	104.18 (14)	H221—C22—H222	108.7
C6—C7—H71	110.6	C22—C23—C24	114.80 (18)
C8—C7—H71	107.3	C22—C23—H231	109.9
C11—C7—H71	110.2	C24—C23—H231	107.5
C7—C8—N9	108.58 (16)	C22—C23—H232	109.2
C7—C8—O26	128.12 (18)	C24—C23—H232	107.4

N9—C8—O26	123.30 (18)	H231—C23—H232	107.7
N9—C10—O28	124.61 (19)	C23—C24—C25	112.1 (2)
N9—C10—C11	108.79 (16)	C23—C24—H241	109.2
O28—C10—C11	126.6 (2)	C25—C24—H241	108.8
C7—C11—C10	104.88 (15)	C23—C24—H242	106.9
C7—C11—C12	113.53 (14)	C25—C24—H242	109.2
C10—C11—C12	109.23 (16)	H241—C24—H242	110.5
C7—C11—H111	111.2	C24—C25—H251	110.7
C10—C11—H111	107.7	C24—C25—H252	110.7
C12—C11—H111	110.0	H251—C25—H252	110.4
C11—C12—C13	111.12 (15)	C24—C25—H253	109.6
C11—C12—H121	109.4	H251—C25—H253	109.2
C13—C12—H121	111.1	H252—C25—H253	106.1
C11—C12—H122	108.2	N9—C27—H271	109.2
C13—C12—H122	109.9	N9—C27—H272	109.7
H121—C12—H122	107.0	H271—C27—H272	112.3
C12—C13—C14	115.99 (16)	N9—C27—H273	107.0
C12—C13—C29	120.82 (15)	H271—C27—H273	109.0
C14—C13—C29	123.18 (17)	H272—C27—H273	109.5
C6—C14—C13	117.84 (15)	N9—C27—H274	109.4
C6—C14—C15	115.70 (14)	N9—C27—H275	109.5
C13—C14—C15	126.43 (16)	H274—C27—H275	109.5
C14—C15—C16	110.11 (14)	N9—C27—H276	109.5
C14—C15—H151	109.3	H274—C27—H276	109.5
C16—C15—H151	108.5	H275—C27—H276	109.5
C14—C15—H152	112.5	C13—C29—C30	127.1 (2)
C16—C15—H152	109.7	C13—C29—H291	116.3
H151—C15—H152	106.6	C30—C29—H291	116.6
C4—C16—C15	113.44 (14)	C29—C30—H301	119.9
C4—C16—C1	104.91 (14)	C29—C30—H302	121.8
C15—C16—C1	109.20 (14)	H301—C30—H302	118.3
O17—C1—N2—C3	178.5 (2)	C5—C6—C7—C8	−64.0 (2)
O17—C1—N2—C18	−0.8 (3)	C5—C6—C7—C11	179.1 (1)
O17—C1—C16—C4	178.7 (2)	C5—C6—C14—C13	−178.0 (1)
O17—C1—C16—C15	−59.4 (2)	C5—C6—C14—C15	4.1 (2)
O19—C3—N2—C1	−177.4 (2)	C5—C20—C21—C22	−174.5 (2)
O19—C3—N2—C18	1.8 (3)	C6—C5—C4—C16	−57.1 (2)
O19—C3—C4—C5	52.6 (2)	C6—C5—C20—C21	−173.6 (1)
O19—C3—C4—C16	176.2 (2)	C6—C7—C11—C10	126.6 (2)
O26—C8—N9—C10	−176.1 (2)	C6—C7—C11—C12	7.4 (2)
O26—C8—N9—C27	3.2 (3)	C6—C14—C13—C12	−0.5 (2)
O26—C8—C7—C6	54.5 (3)	C6—C14—C13—C29	−179.4 (2)
O26—C8—C7—C11	175.3 (2)	C6—C14—C15—C16	−53.2 (2)
O28—C10—N9—C8	178.1 (2)	C7—C6—C5—C20	−58.3 (2)
O28—C10—N9—C27	−1.2 (3)	C7—C6—C14—C13	52.5 (2)
O28—C10—C11—C7	178.3 (2)	C7—C6—C14—C15	−125.4 (2)
O28—C10—C11—C12	−59.7 (3)	C7—C8—N9—C10	4.6 (2)
N2—C1—C16—C4	−2.5 (2)	C7—C8—N9—C27	−176.1 (2)
N2—C1—C16—C15	119.4 (2)	C7—C11—C12—C13	43.0 (2)

N2—C3—C4—C5	−128.0 (2)	C8—N9—C10—C11	−1.6 (2)
N2—C3—C4—C16	−4.4 (2)	C8—C7—C6—C14	63.6 (2)
N9—C8—C7—C6	−126.3 (2)	C8—C7—C11—C10	4.3 (2)
N9—C8—C7—C11	−5.4 (2)	C8—C7—C11—C12	−114.8 (2)
N9—C10—C11—C7	−1.9 (2)	C10—C11—C12—C13	−73.7 (2)
N9—C10—C11—C12	120.1 (2)	C11—C7—C6—C14	−53.3 (2)
C1—N2—C3—C4	3.1 (2)	C11—C10—N9—C27	179.0 (2)
C1—C16—C4—C3	4.1 (2)	C11—C12—C13—C14	−48.7 (2)
C1—C16—C4—C5	128.1 (2)	C11—C12—C13—C29	130.2 (2)
C1—C16—C15—C14	−71.3 (2)	C12—C13—C14—C15	177.1 (2)
C3—N2—C1—C16	−0.3 (2)	C12—C13—C29—C30	−14.9 (3)
C3—C4—C5—C6	61.5 (2)	C13—C14—C15—C16	129.1 (2)
C3—C4—C5—C20	−64.2 (2)	C14—C6—C5—C20	176.6 (1)
C3—C4—C16—C15	−115.0 (2)	C14—C13—C29—C30	163.9 (2)
C4—C3—N2—C18	−177.6 (2)	C15—C14—C13—C29	−1.7 (3)
C4—C5—C6—C7	175.4 (1)	C16—C1—N2—C18	−179.6 (2)
C4—C5—C6—C14	50.3 (2)	C16—C4—C5—C20	177.2 (1)
C4—C5—C20—C21	−50.3 (2)	C20—C21—C22—C23	179.8 (2)
C4—C16—C15—C14	45.3 (2)	C21—C22—C23—C24	−74.7 (2)
C5—C4—C16—C15	9.0 (2)	C22—C23—C24—C25	−179.4 (2)

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