4'-(1-(4-Methoxyphenyl)-4-oxo-3-phenyl azetidin-2-yl)-1'-methyl-2-oxo-2H- spiro [acenaphthylene-1,2'-pyrrolidine]-3',3'-dicarbonitrile

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ABSTRACT

In the title compound, $C_{34}H_{26}N_4O_3 1.5H_2O$, β_ lactam ring is essentially planar, with the O atom displaced from this plane by- 0.053 (1) A ° , and forming dihedral angles of 39.71(8) and 79.32(9) with the planes of the benzene substituent groups on this ring. The pyrolidine ring adopts an envelope conformation. In the crystal, The crystal packing of the molecules of compound II is stabilized by the weak C-H…N interactions.

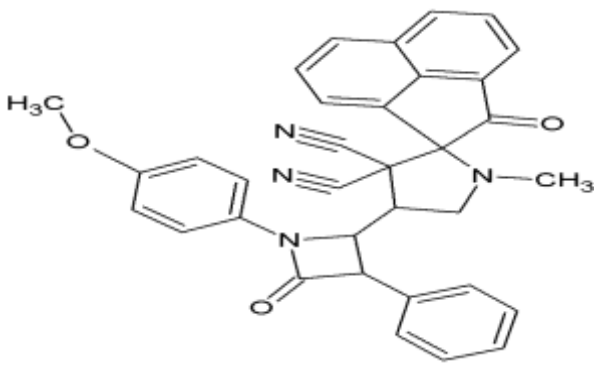
Keywords: *β_ lactam, pyrolidine ring single-crystal X-ray study.*

1.INTRODUCTION

A **β-lactam** (**beta-lactam**) ring is a four-membered cyclic amide. It is named as such because the nitrogen atom is attached to the β-carbon relative to the carbonyl. The simplest β-lactam possible is 2-azetidinone. Though the first member was synthesized by Staudinger in1907, the Beta lactams as a class acquired importance since the discovery of penicillin which contains Beta lactam unit as an essential structural feature of its molecule. This interest continued unabated because of the therapeutic importance of Beta lactam antibiotics

A large number of monocyclic β- lactams possess powerful antibacterial, antimicrobial, anti-inflammatory, anti-convulsant, anti-viral, herbicidal antitubercular activity etc. β -lactam derivatives containing natural gallic acid moiety have evaluated with biological properties as potential agricultural protective plant agents.

The present work is undertaken to explore more possibilities of finding a suitable derivatives, which would exceed its activity more than the already known drugs containing β-lactam ring. X-ray crystallographic studies of the compound has been carried out.



Crystal data

$C_{34}H_{26}N_4O_3 1.5H_2O$	V = 1527.1(12)Å³
Mr = 565.61	Z = 2
Triclinic, Pī	Mo K_ radiation
a = 9.004(5) Å	$\mu = 1.58\ mm^{-1}$
b = 9.806(5) Å	T = 293 K
c = 17.735(5) Å	0.25 × 0.20 ×0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi -scan(SADABS; Bruker 2008)
Tmin = 0.979, Tmax = 0.983

7712 independen t reflections
5355 reflections with I> 2_(I)
Rint = 0.062

Refinement

R[F2 > 2_(F2)] = 0.062
wR(F2) = 0.192
S = 1.09
7712 reflections
417 parameters
49 restraint
H-atom parameters constrained
__max = 0.84 e A ° _3
__min = _0.22 e A ° _3
Absolute structure: Flack (1983), 2910 Friedel pairs
Absolute structure parameter: 0.006 (5)

Data collection:

APEX2 (Bruker, 2008); cell refinement: APEX2 and SAINT (Bruker, 2008); data reduction: SAINT and XPREP (Bruker, 2008); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012); software used to prepare material for publication:
PLATON (Spek, 2009).

2.COMMENT

The most commonly used *β*-lactam antibiotics for the therapy of infectious diseases are penicillin and cephalosporin(Brakhage, 1998). In view of potential applications, the crystal structure determination of the title *β*-lactam derivative, $C_{34}H_{26}N_4O_3 1.5H_2O$, was carried out and is reported herein. In this compound, the four-membered ring of the *β*-lactam fragment (N2/C1–C3) is essentially planar (r.m.s. deviation = 0.0122 A), with O1 displaced from the plane by - 0.053 (1) A°. The mean-planes of the benzene rings of the two benzene substituent groups defined by C4–C9 and C10–C15 areinclined at dihedral angles 39.71(8) and 79.32(9)° respectively, with respect to four-membered *β*-lactam ring. The pyrrolidine ring (N1/C16-C19) adopts an envelope conformation, defined by the asymmetry parameters (Nardelli, 1983), DS(N2) = 8.09(10) and D2 (C16) = 2.33 (8) respectively. the acenaphthylene moiety is planar and is almost perpendicular to the attached pyrrolidine moiety with a dihedral angle of 88.33(7)°. Atom O3 deviates by 0.109(1) Å from the least-squares plane of the acenaphthylene ring. The 1.5 water molecules in the void are disordered with the atoms O1W, O2W, O3W, O4W and O5W with site occupancies of 0.5, 0.25, 0.31, 0.41 and 0.23 respectively.

The crystal packing of the molecules of compound II is stabilized by the weak C-H…N interactions. The molecular conformation is stabilized by week intra-molecular C-H…O hydrogen bonds.

3.EXPERIMENTAL

To a reaction mixture of 2-((1-(4-methoxyphenyl)-4-oxo-3-phenylazetidin-2-yl) methylene)malononitrile (1 mmol), acenapthenequinone (1 mmol) and sarcosine (1.1 mmol) was refluxed in methanol until completion of the reaction was evidenced by TLC analysis. After completion of the reaction the solvent was evaporated under reduced pressure. The crude reaction mixture was dissolved in dichloromethane and washed with water followed by brine solution. The organic layer was separated and dried over sodium sulfate, filtering and evaporation of the organic solvent under reduced pressure. The product was separated by column chromatography using hexane and ethyl acetate (3:7) as an eluent to give yellow solid. The product was dissolved in ethyl acetate and heated for two minutes. The resulting solution was subjected to crystallization by slow evaporation of the solvent resulting in single crystals suitable for XRD studies

3.1Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *APEX2* and *SAINT* (Bruker, 2008); data reduction: *SAINT* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009).

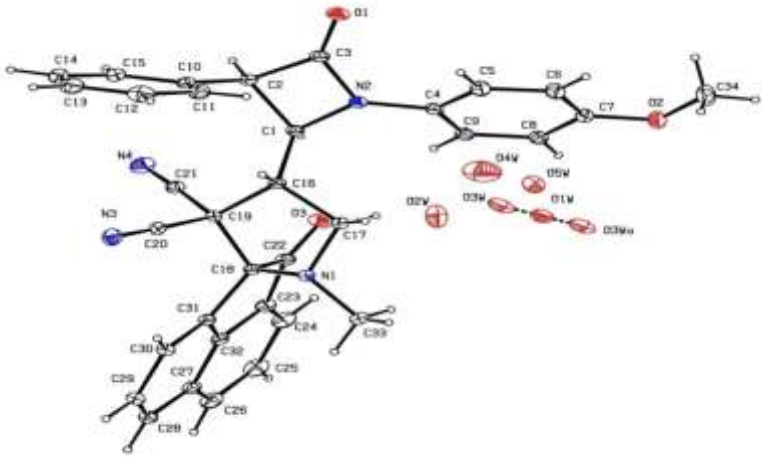


Figure 1

The molecular configuration and atom numbering for the title compound, with displacement ellipsoids drawn at the 30% probability level

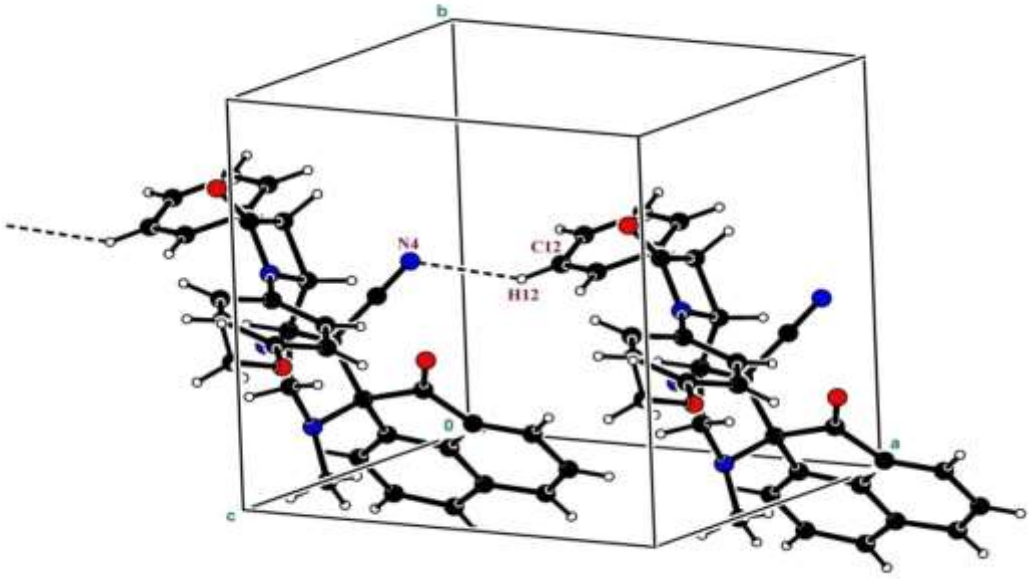


Figure 2
The crystal packing of the title compound, with hydrogen bonds shown as dashed lines. H-atoms not involved in interactions have been omitted.

Parameters	
Empirical formula	$C_{34}H_{26}N_4O_3 1.5H_2O$
Formula weight	565.61
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	Pī
Unit cell dimensions	a = 9.004(5) Å
	b = 9.806(5) Å
	c = 17.735(5) Å
	α = 93.668(5)°
	β = 99.161(5)°
	γ = 97.443(5)°
Volume	1527.1(12) Å^3
Z, Calculated density	2, 1.230 Mg/m^3
Absorption coefficient	0.083 mm^{-1}

F(000)	594
Crystal size(mm)	0.25 x 0.25 x 0.20
θ range	1.17 to 28.53°
Limiting indices	$-12 \leq h \leq 12$,
	$-13 \leq k \leq 13$,
	$-23 \leq l \leq 23$
Reflections collected / unique	32374 / 7712 [R(int) = 0.031]
Completeness to theta	99.50%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7712/49/ 417
Goodness-of-fit on F^2	1.09
Final R indices [I>2σ(I)]	R1 = 0.062
R indices (all data)	wR2 = 0.192
	R1 = 0.094
	wR2 = 0.220
Largest diff. peak and hole	0.84 and -0.22 e.$Å^{-3}$

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

Atom	**x**	**y**	**z**	***U(eq)**
C1	7875(2)	4028(2)	2990(1)	39(1)
C2	7208(2)	5366(2)	2741(1)	43(1)
C3	6824(2)	5489(2)	3548(1)	49(1)
C4	7811(2)	3838(2)	4466(1)	43(1)
C5	6850(3)	3883(3)	4997(1)	57(1)
C6	7281(3)	3534(3)	5735(1)	61(1)
C7	8680(3)	3111(2)	5939(1)	51(1)
C8	9626(2)	3023(2)	5402(1)	49(1)
C9	9213(2)	3395(2)	4677(1)	46(1)
C10	5917(2)	5304(2)	2092(1)	46(1)
C11	4472(3)	4680(3)	2150(2)	59(1)
C12	3279(3)	4641(3)	1549(2)	79(1)
C13	3503(4)	5249(3)	899(2)	90(1)
C14	4919(5)	5895(3)	838(2)	83(1)
C15	6131(3)	5912(2)	1429(1)	61(1)

C16	7134(2)	2658(2)	2565(1)	38(1)
C17	7369(3)	1405(2)	3017(1)	47(1)
C18	8550(2)	1001(2)	1955(1)	38(1)
C19	7746(2)	2310(2)	1799(1)	36(1)
C20	6465(2)	1994(2)	1161(1)	43(1)
C21	8757(2)	3455(2)	1566(1)	45(1)
C22	10247(2)	1459(2)	2360(1)	47(1)
C23	11209(2)	650(2)	1972(1)	50(1)
C24	12729(3)	561(3)	2115(2)	64(1)
C25	13307(3)	-338(3)	1637(2)	74(1)
C26	12395(3)	-1126(3)	1033(2)	73(1)
C27	10808(3)	-1076(2)	866(1)	55(1)
C28	9726(3)	-1836(2)	282(1)	65(1)
C29	8233(3)	-1663(2)	214(1)	61(1)
C30	7696(3)	-740(2)	723(1)	49(1)
C31	8720(2)	22(2)	1283(1)	41(1)
C32	10264(2)	-149(2)	1353(1)	45(1)
C33	8062(3)	-879(2)	2790(1)	61(1)
C34	8326(4)	2907(4)	7230(2)	89(1)
N1	7562(2)	336(2)	2449(1)	42(1)
N2	7381(2)	4297(2)	3735(1)	45(1)
N3	5487(2)	1788(2)	658(1)	66(1)
N4	9485(2)	4330(2)	1351(1)	69(1)
O1	6269(2)	6309(2)	3909(1)	68(1)
O2	9222(2)	2758(2)	6651(1)	70(1)
O3	10636(2)	2318(2)	2895(1)	72(1)
O1W	5000	0000	5000	72(2)
O2W	14422(8)	393(9)	3946(4)	93(3)
O3W	4274(11)	289(9)	4632(5)	78(2)
O4W	12637(10)	846(9)	4567(7)	162(4)
O5W	3468(15)	460(10)	5035(6)	90(4)

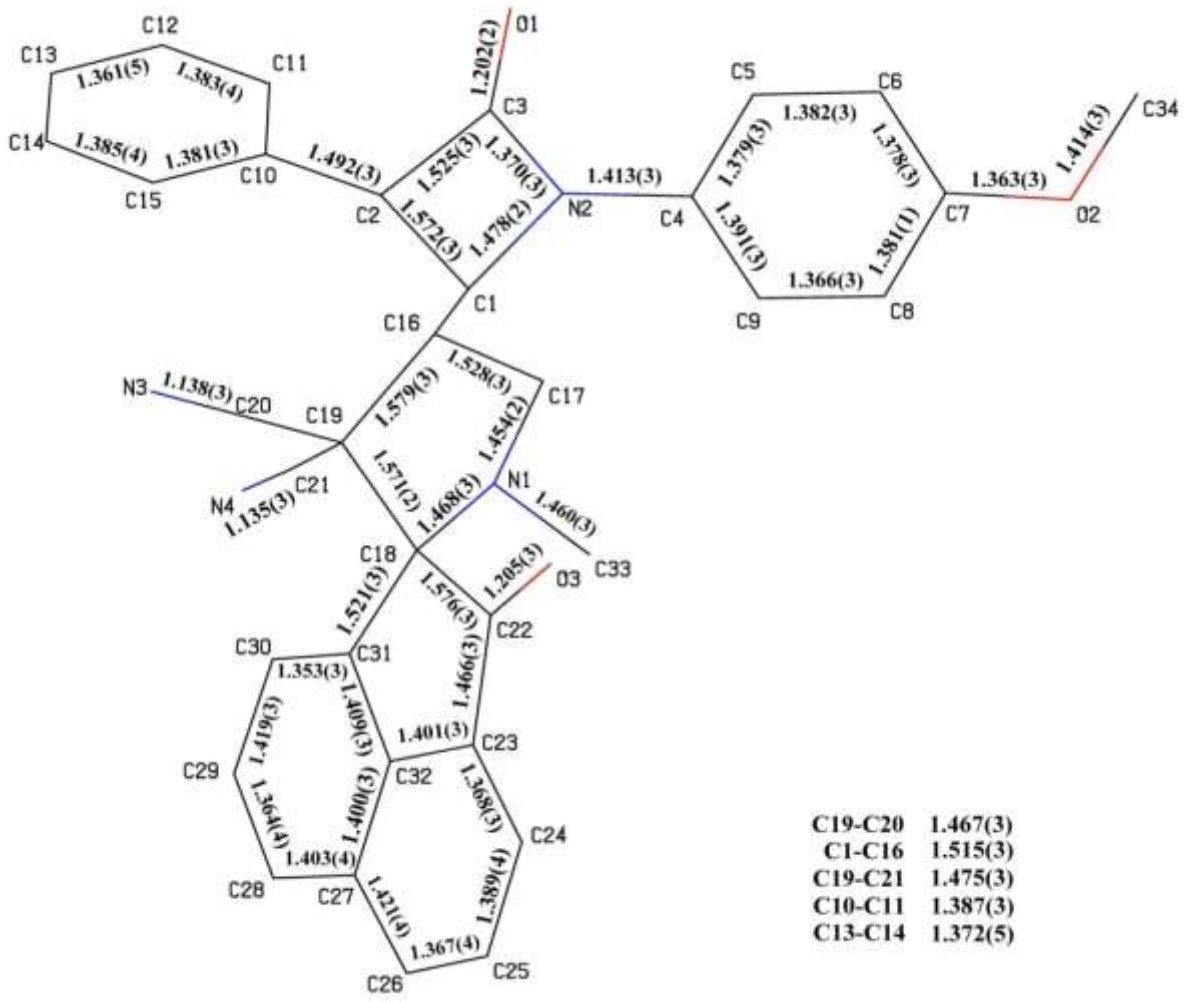
Atomic displacement parameters $Å^2$

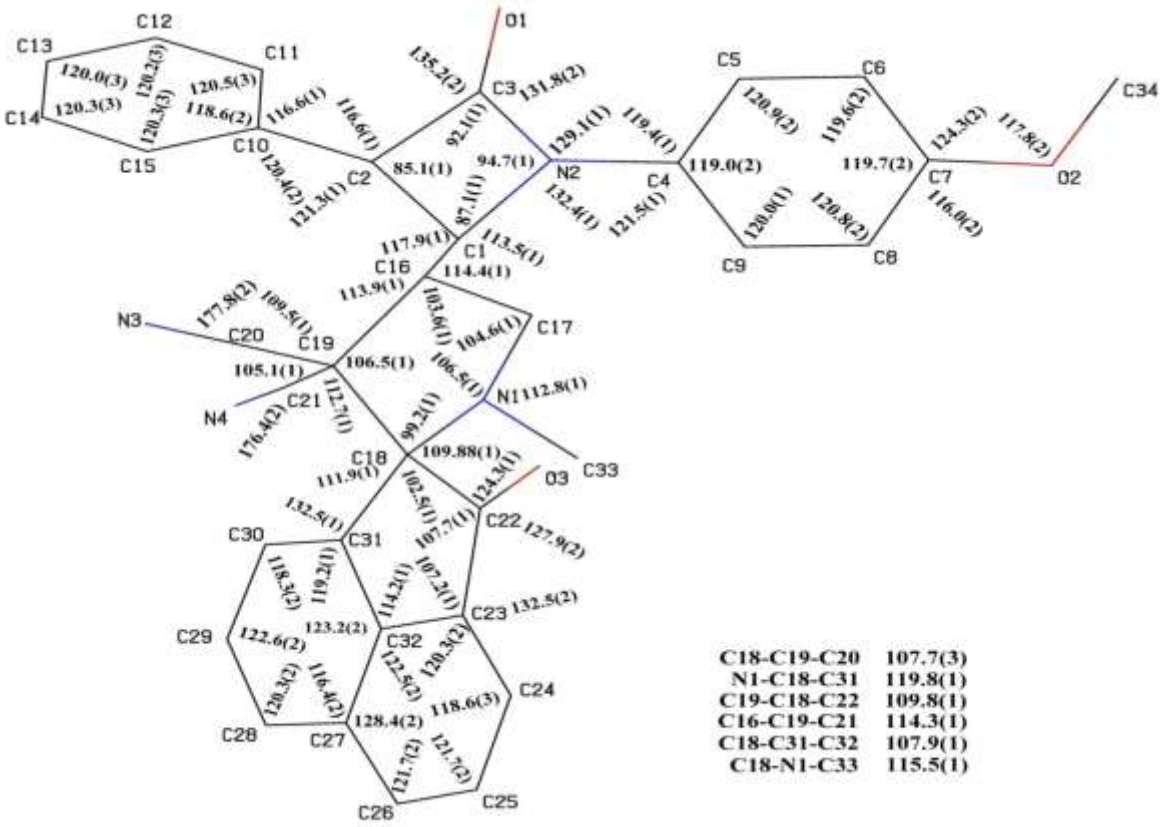
Atom	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
C1	41(1)	35(1)	43(1)	-1(1)	7(1)	11(1)
C2	44(1)	31(1)	54(1)	0(1)	6(1)	10(1)

C3	51(1)	41(1)	54(1)	-6(1)	2(1)	18(1)
C4	47(1)	40(1)	42(1)	-5(1)	5(1)	13(1)
C5	50(1)	71(2)	56(1)	4(1)	12(1)	25(1)
C6	61(1)	74(2)	55(1)	7(1)	21(1)	26(1)
C7	58(1)	50(1)	44(1)	2(1)	7(1)	15(1)
C8	46(1)	51(1)	50(1)	-2(1)	3(1)	17(1)
C9	44(1)	48(1)	47(1)	-4(1)	9(1)	13(1)
C10	53(1)	35(1)	51(1)	1(1)	5(1)	17(1)
C11	51(1)	59(1)	69(2)	2(1)	8(1)	19(1)
C12	52(2)	78(2)	100(2)	-11(2)	-9(1)	24(1)
C13	99(3)	74(2)	85(2)	-16(2)	-35(2)	42(2)
C14	129(3)	59(2)	58(2)	6(1)	-10(2)	32(2)
C15	82(2)	42(1)	59(1)	6(1)	7(1)	15(1)
C16	41(1)	33(1)	42(1)	1(1)	11(1)	11(1)
C17	66(1)	36(1)	43(1)	4(1)	14(1)	15(1)
C18	41(1)	33(1)	41(1)	-1(1)	4(1)	12(1)
C19	37(1)	31(1)	40(1)	2(1)	8(1)	8(1)
C20	47(1)	40(1)	43(1)	6(1)	6(1)	12(1)
C21	45(1)	40(1)	52(1)	4(1)	14(1)	11(1)
C22	44(1)	39(1)	57(1)	-2(1)	0(1)	14(1)
C23	46(1)	42(1)	66(1)	10(1)	14(1)	14(1)
C24	43(1)	58(1)	94(2)	18(1)	14(1)	14(1)
C25	52(1)	78(2)	106(2)	31(2)	34(2)	29(1)
C26	84(2)	71(2)	87(2)	29(2)	52(2)	42(2)
C27	72(2)	48(1)	57(1)	16(1)	32(1)	27(1)
C28	105(2)	50(1)	51(1)	5(1)	34(1)	31(1)
C29	94(2)	45(1)	45(1)	-4(1)	12(1)	14(1)
C30	63(1)	41(1)	45(1)	-2(1)	9(1)	12(1)
C31	51(1)	33(1)	43(1)	3(1)	12(1)	13(1)
C32	53(1)	39(1)	51(1)	11(1)	19(1)	17(1)
C33	94(2)	36(1)	58(1)	8(1)	13(1)	21(1)
C34	106(2)	117(3)	54(2)	21(2)	28(2)	29(2)
N1	56(1)	30(1)	40(1)	2(1)	8(1)	10(1)
N2	53(1)	43(1)	44(1)	-3(1)	8(1)	22(1)
N3	65(1)	70(1)	58(1)	7(1)	-9(1)	12(1)
N4	62(1)	56(1)	95(2)	14(1)	31(1)	4(1)
O1	81(1)	61(1)	67(1)	-13(1)	7(1)	39(1)
O2	82(1)	86(1)	48(1)	12(1)	10(1)	31(1)
O3	55(1)	65(1)	86(1)	-29(1)	-17(1)	20(1)
O1W	82(4)	61(3)	65(4)	-22(3)	-11(3)	22(3)
O2W	78(4)	139(6)	68(4)	22(4)	13(3)	26(4)
O3W	99(6)	58(4)	76(5)	-27(4)	45(5)	-17(4)
O4W	149(6)	137(6)	194(8)	-33(5)	3(6)	54(5)

O5W	124(6)	75(5)	63(5)	-6(4)	-2(5)	12(4)

Geometric parameters(Å ,°)

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C13
C11
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C10
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C2
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N2
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C6
C7
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O2
C34
C1
C16
C17
C19
C20
N3
C21
N4
C18
N1
C33
O3
C22
C23
C30
C31
C29
C32
C24
C28
C27
C26
C25
C18-C19-C20 107.7(3)
N1-C18-C31 119.8(1)
C19-C18-C22 109.8(1)
C16-C19-C21 114.3(1)
C18-C31-C32 107.9(1)
C18-N1-C33 115.5(1)

Torsional angles

Atoms	Angle	Atoms	Angle
N(2)-C(1)-C(2)-C(10)	-117.0 (2)	N(1)-C(18)-C(22)-C(23)	115.55 (18)
C(16)-C(1)-C(2)-C(10)	-1.8 (3)	C(31)-C(18)-C(22)-C(23)	-5.8 (2)
N(2)-C(1)-C(2)-C(3)	1.36 (14)	C(19)-C(18)-C(22)-C(23)	-133.91 (17)
C(16)-C(1)-C(2)-C(3)	116.60 (18)	O(3)-C(22)-C(23)-C(24)	4.5 (4)
C(10)-C(2)-C(3)-O(1)	-59.7 (3)	C(18)-C(22)-C(23)-C(24)	-175.0 (2)
C(1)-C(2)-C(3)-O(1)	177.4 (3)	O(3)-C(22)-C(23)-C(32)	-176.3 (2)
C(10)-C(2)-C(3)-N(2)	121.38 (18)	C(18)-C(22)-C(23)-C(32)	4.2 (2)
C(1)-C(2)-C(3)-N(2)	-1.47 (16)	C(32)-C(23)-C(24)-C(25)	-0.1 (3)
C(9)-C(4)-C(5)-C(6)	1.9 (4)	C(22)-C(23)-C(24)-C(25)	179.0 (2)
N(2)-C(4)-C(5)-C(6)	-175.4 (2)	C(23)-C(24)-C(25)-C(26)	-0.1 (4)
C(4)-C(5)-C(6)-C(7)	-1.2 (4)	C(24)-C(25)-C(26)-C(27)	-0.5 (4)
C(5)-C(6)-C(7)-O(2)	179.3 (2)	C(25)-C(26)-C(27)-C(32)	1.2 (3)
C(5)-C(6)-C(7)-C(8)	-0.9 (4)	C(25)-C(26)-C(27)-C(28)	-178.6 (2)
O(2)-C(7)-C(8)-C(9)	-177.9 (2)	C(32)-C(27)-C(28)-C(29)	-0.7 (3)
C(6)-C(7)-C(8)-C(9)	2.3 (4)	C(26)-C(27)-C(28)-C(29)	179.1 (2)
C(7)-C(8)-C(9)-C(4)	-1.5 (3)	C(27)-C(28)-C(29)-C(30)	-0.6 (4)
C(5)-C(4)-C(9)-C(8)	-0.5 (3)	C(28)-C(29)-C(30)-C(31)	1.7 (3)
N(2)-C(4)-C(9)-C(8)	176.68 (19)	C(29)-C(30)-C(31)-C(32)	-1.4 (3)
C(3)-C(2)-C(10)-C(15)	144.9 (2)	C(29)-C(30)-C(31)-C(18)	-174.1 (2)
C(1)-C(2)-C(10)-C(15)	-113.8 (2)	N(1)-C(18)-C(31)-C(30)	55.7 (3)
C(3)-C(2)-C(10)-C(11)	-32.8 (3)	C(19)-C(18)-C(31)-C(30)	-59.6 (3)
C(1)-C(2)-C(10)-C(11)	68.5 (3)	C(22)-C(18)-C(31)-C(30)	178.6 (2)
C(15)-C(10)-C(11)-C(12)	1.6 (3)	N(1)-C(18)-C(31)-C(32)	-117.57 (17)
C(2)-C(10)-C(11)-C(12)	179.3 (2)	C(19)-C(18)-C(31)-C(32)	127.08 (18)
C(10)-C(11)-C(12)-C(13)	-1.8 (4)	C(22)-C(18)-C(31)-C(32)	5.35 (19)
C(11)-C(12)-C(13)-C(14)	0.5 (4)	C(28)-C(27)-C(32)-C(23)	178.4 (2)
C(12)-C(13)-C(14)-C(15)	1.1 (4)	C(26)-C(27)-C(32)-C(23)	-1.4 (3)
C(11)-C(10)-C(15)-C(14)	0.0 (3)	C(28)-C(27)-C(32)-C(31)	1.0 (3)
C(2)-C(10)-C(15)-C(14)	-177.7 (2)	C(26)-C(27)-C(32)-C(31)	-178.85 (19)
C(13)-C(14)-C(15)-C(10)	-1.4 (4)	C(24)-C(23)-C(32)-C(27)	0.9 (3)

Contd…..

Atoms	Angle	Atoms	Angle
N(2)-C(1)-C(16)-C(17)	-56.6 (2)	C(22)-C(23)-C(32)-C(27)	-178.40 (18)
C(2)-C(1)-C(16)-C(17)	-156.30 (17)	C(24)-C(23)-C(32)-C(31)	178.6 (2)
N(2)-C(1)-C(16)-C(19)	-175.61 (15)	C(22)-C(23)-C(32)-C(31)	-0.8 (2)
C(2)-C(1)-C(16)-C(19)	84.7 (2)	C(30)-C(31)-C(32)-C(27)	0.1 (3)
N(1)-C(17)-C(16)-C(1)	-142.48 (17)	C(18)-C(31)-C(32)-C(27)	174.45 (18)
N(1)-C(17)-C(16)-C(19)	-17.8 (2)	C(30)-C(31)-C(32)-C(23)	-177.54 (19)
C(1)-C(16)-C(19)-C(20)	-126.40 (17)	C(18)-C(31)-C(32)-C(23)	-3.2 (2)
C(17)-C(16)-C(19)-C(20)	108.63 (17)	O(1)-C(3)-N(2)-C(4)	-17.2 (4)
C(1)-C(16)-C(19)-C(21)	-8.7 (2)	C(2)-C(3)-N(2)-C(4)	161.8 (2)
C(17)-C(16)-C(19)-C(21)	-133.68 (18)	O(1)-C(3)-N(2)-C(1)	-177.4 (3)
C(1)-C(16)-C(19)-C(18)	114.90 (17)	C(2)-C(3)-N(2)-C(1)	1.56 (16)
C(17)-C(16)-C(19)-C(18)	-10.06 (19)	C(5)-C(4)-N(2)-C(3)	48.0 (3)
C(21)-C(19)-C(20)-N(3)	-12 (6)	C(9)-C(4)-N(2)-C(3)	-129.2 (2)
C(18)-C(19)-C(20)-N(3)	-135 (6)	C(5)-C(4)-N(2)-C(1)	-159.3 (2)
C(16)-C(19)-C(20)-N(3)	111 (6)	C(9)-C(4)-N(2)-C(1)	23.6 (3)
C(20)-C(19)-C(21)-N(4)	-5 (4)	C(16)-C(1)-N(2)-C(3)	-120.82 (18)
C(18)-C(19)-C(21)-N(4)	116 (3)	C(2)-C(1)-N(2)-C(3)	-1.52 (16)
C(16)-C(19)-C(21)-N(4)	-125 (3)	C(16)-C(1)-N(2)-C(4)	80.0 (3)
C(20)-C(19)-C(18)-N(1)	-84.24 (17)	C(2)-C(1)-N(2)-C(4)	-160.7 (2)
C(21)-C(19)-C(18)-N(1)	158.19 (16)	C(16)-C(17)-N(1)-C(33)	170.06 (18)
C(16)-C(19)-C(18)-N(1)	33.55 (17)	C(16)-C(17)-N(1)-C(18)	42.3 (2)
C(20)-C(19)-C(18)-C(31)	37.6 (2)	C(31)-C(18)-N(1)-C(17)	-174.33 (16)
C(21)-C(19)-C(18)-C(31)	-79.9 (2)	C(19)-C(18)-N(1)-C(17)	-47.17 (18)
C(16)-C(19)-C(18)-C(31)	155.44 (16)	C(22)-C(18)-N(1)-C(17)	69.67 (19)
C(20)-C(19)-C(18)-C(22)	155.65 (16)	C(31)-C(18)-N(1)-C(33)	59.4 (2)
C(21)-C(19)-C(18)-C(22)	38.1 (2)	C(19)-C(18)-N(1)-C(33)	-173.40 (17)
C(16)-C(19)-C(18)-C(22)	-86.55 (18)	C(22)-C(18)-N(1)-C(33)	-56.6 (2)
N(1)-C(18)-C(22)-O(3)	-63.9 (3)	C(6)-C(7)-O(2)-C(34)	-3.6 (4)
C(31)-C(18)-C(22)-O(3)	174.7 (2)	C(8)-C(7)-O(2)-C(34)	176.6 (2)
C(19)-C(18)-C(22)-O(3)	46.6 (3)		

Hydrogen bond interactions[Å and º]

Compounds	D-H…A	D-H	H…A	D…A	D-H…A
II	C12-H12…N4[i]	0.93	2.53	3.350(3)	145

Symmetry Codes:	
Compound II:	(i) -1+x, y, z

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