Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C14 H21 N9 O6 COMPOUND (bent52)

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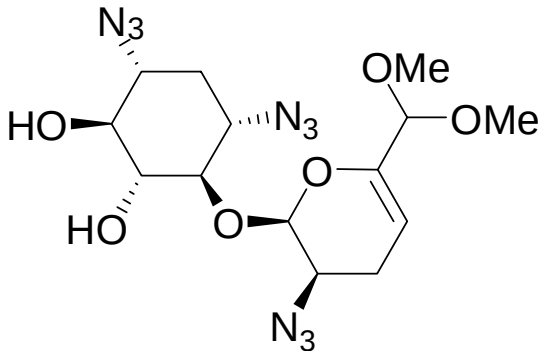

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C14 H21 N9 O6.

Identification code	bent52
Empirical formula	C14 H21 N9 O6
Formula weight	411.40
Temperature	150K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 15.8942(5) Å α = 89.7480(10)° b = 16.2322(5) Å β = 72.741(2)° c = 17.6688(6) Å γ = 63.5370(10)°
Volume	3853.3(2)Å^3
Z	8
Density (calculated)	1.418 g/cm^3
Absorption coefficient	0.966 mm^{-1}
F(000)	1728
Crystal size	0.36 x 0.25 x 0.06 mm
Theta range for data collection	2.65 to 64.12°
Index ranges	$-17 \le h \le 18$, $-18 \le k \le 18$, $-20 \le \ell \le 19$
Reflections collected	53806
Independent reflections	20234 [R_{int} = 0.033]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9437 and 0.8116
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	20234 / 447 / 2194
Goodness-of-fit on F^2	0.985
Final R indices [I>2sigma(I)]	R_1 = 0.0440, wR_2 = 0.1069
R indices (all data)	R_1 = 0.0536, wR_2 = 0.1117
Absolute structure parameter	0.10(11)

Extinction coefficient	0.00085(6)
Largest diff. peak and hole	0.357 and -0.265 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C14 H21 N9 O6.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
O(11)	1	8350(2)	1208(2)	10406(1)	35(1)
O(12)	1	9427(2)	1792(2)	9735(2)	37(1)
O(13)	1	7734(2)	1409(2)	9036(1)	28(1)
O(14)	1	7818(2)	254(2)	8181(1)	27(1)
O(15)	1	5741(2)	1254(2)	8224(2)	32(1)
O(16)	1	4876(2)	102(2)	8092(1)	31(1)
N(11)	1	8095(2)	1120(2)	6842(2)	37(1)
N(12)	1	8641(3)	303(3)	6519(2)	46(1)
N(13)	1	9077(3)	-434(3)	6191(3)	69(1)
N(14)	1	5362(2)	-1502(2)	8975(2)	35(1)
N(15)	1	4821(2)	-1541(2)	8639(2)	32(1)
N(16)	1	4260(2)	-1627(2)	8413(2)	40(1)
N(17)	1	8212(2)	-1207(2)	9125(2)	37(1)
N(18)	1	9073(3)	-1373(2)	8757(2)	43(1)
N(19)	1	9880(3)	-1529(3)	8490(3)	76(1)
C(11)	1	8548(3)	1747(3)	9810(2)	30(1)
C(12)	1	8619(2)	1397(3)	8989(2)	30(1)
C(13)	1	9393(2)	1146(3)	8333(2)	32(1)
C(14)	1	9350(3)	856(3)	7540(2)	34(1)
C(15)	1	8285(3)	1354(3)	7571(2)	30(1)
C(16)	1	7598(3)	1192(2)	8300(2)	25(1)
C(17)	1	7029(2)	39(2)	8607(2)	24(1)
C(18)	1	6265(3)	274(2)	8181(2)	26(1)
C(19)	1	5524(3)	-100(3)	8557(2)	29(1)
C(110)	1	6066(3)	-1138(3)	8566(2)	30(1)
C(111)	1	6794(3)	-1346(2)	9022(2)	28(1)
C(112)	1	7547(3)	-1000(2)	8636(2)	29(1)
C(113)	1	9062(3)	240(3)	10227(3)	50(1)
C(114)	1	9363(3)	2335(3)	10401(2)	50(1)
O(21)	1	9471(2)	5002(2)	10022(2)	38(1)
O(22)	1	8067(2)	6447(2)	10490(2)	37(1)
O(23)	1	7735(2)	6246(2)	9028(1)	31(1)
O(24)	1	7800(2)	5194(2)	8088(1)	28(1)
O(25)	1	5777(2)	6239(2)	8115(2)	37(1)
O(26)	1	4893(2)	5076(2)	7943(1)	35(1)
N(22A)	0.49	8867(5)	5360(4)	6417(4)	53(2)
N(23A)	0.49	9242(6)	4684(4)	5985(4)	74(2)
N(32A)	0.49	8915(4)	2910(6)	6518(4)	43(2)
N(33A)	0.49	9523(4)	2837(6)	6767(4)	68(2)
C(63A)	0.49	1626(6)	8530(20)	5700(7)	45(5)
C(64A)	0.49	1654(7)	8450(20)	4832(6)	62(3)
C(65A)	0.49	2667(8)	7703(14)	4294(6)	71(2)
C(66A)	0.49	3488(7)	7809(5)	4500(4)	51(1)
N(61A)	0.49	2905(7)	7676(8)	3418(5)	83(2)
N(62A)	0.49	2244(6)	8038(5)	3139(4)	71(2)
N(63A)	0.49	1708(6)	8278(6)	2782(5)	88(2)
N(82A)	0.49	2439(4)	10488(4)	3110(4)	48(2)
N(83A)	0.49	2003(5)	10123(6)	3439(4)	75(2)
N(88A)	0.49	2207(2)	8877(6)	563(4)	47(2)

N(89A)	0.49	1375(3)	9134(7)	711(5)	76(2)
N(22B)	0.51	9023(4)	5652(5)	6229(3)	53(2)
N(23B)	0.51	9561(4)	5274(6)	5607(3)	74(2)
N(32B)	0.51	8733(4)	3324(4)	6391(4)	43(2)
N(33B)	0.51	9145(5)	3711(5)	6493(4)	68(2)
C(63B)	0.51	1621(5)	8720(20)	5750(6)	45(5)
C(64B)	0.51	1524(7)	8630(20)	4924(6)	62(3)
C(65B)	0.51	2494(8)	7830(13)	4368(6)	71(2)
C(66B)	0.51	3388(6)	7832(5)	4490(4)	51(1)
N(61B)	0.51	2596(8)	7882(7)	3476(5)	83(2)
N(62B)	0.51	2254(6)	8625(6)	3252(4)	71(2)
N(63B)	0.51	2018(7)	9285(7)	2967(5)	88(2)
N(82B)	0.51	2279(4)	10992(5)	3350(3)	48(2)
N(83B)	0.51	1672(4)	11110(6)	3940(3)	75(2)
N(88B)	0.51	2236(3)	9143(5)	659(4)	47(2)
N(89B)	0.51	1421(3)	9685(5)	904(5)	76(2)
N(21)	1	8360(3)	6107(2)	6834(2)	54(1)
N(24)	1	5244(2)	3575(2)	8977(2)	34(1)
N(25)	1	4692(2)	3516(2)	8638(2)	32(1)
N(26)	1	4131(3)	3408(2)	8428(2)	42(1)
N(27)	1	8087(2)	3847(2)	9158(2)	31(1)
N(28)	1	8988(3)	3513(2)	8775(2)	36(1)
N(29)	1	9828(3)	3209(2)	8493(2)	51(1)
C(21)	1	8545(3)	5590(3)	9968(2)	31(1)
C(22)	1	8663(3)	5714(2)	9102(2)	29(1)
C(23)	1	9500(3)	5331(3)	8491(2)	35(1)
C(24)	1	9526(3)	5409(3)	7634(2)	39(1)
C(25)	1	8535(3)	6145(3)	7601(2)	39(1)
C(26)	1	7684(3)	6090(3)	8246(2)	32(1)
C(27)	1	6986(3)	5038(2)	8544(2)	26(1)
C(28)	1	6240(3)	5261(2)	8099(2)	29(1)
C(29)	1	5466(3)	4931(3)	8470(2)	28(1)
C(210)	1	5967(3)	3904(3)	8549(2)	30(1)
C(211)	1	6637(3)	3744(3)	9055(2)	31(1)
C(212)	1	7449(3)	4014(2)	8649(2)	27(1)
C(213)	1	9403(3)	4693(3)	10793(2)	50(1)
C(214)	1	8569(4)	7004(3)	10336(3)	53(1)
O(31)	1	9290(2)	1361(2)	2744(2)	47(1)
O(32)	1	8130(2)	2871(2)	2749(2)	39(1)
O(33)	1	7657(2)	3082(2)	4443(1)	32(1)
O(34)	1	7850(2)	4131(2)	5181(1)	30(1)
O(35)	1	5781(2)	4974(2)	6252(2)	36(1)
O(36)	1	4993(2)	6881(2)	6852(1)	36(1)
N(31)	1	8201(2)	2992(2)	6355(2)	44(1)
N(34)	1	5486(3)	8020(2)	5662(2)	40(1)
N(35)	1	4920(3)	8545(2)	6313(2)	35(1)
N(36)	1	4361(3)	9114(3)	6843(2)	42(1)
N(37)	1	8239(3)	5228(2)	3995(2)	38(1)
N(38)	1	9092(3)	4594(3)	3897(2)	43(1)
N(39)	1	9883(3)	4027(3)	3719(2)	64(1)
C(31)	1	8427(3)	2122(3)	3190(2)	36(1)
C(32)	1	8555(3)	2387(3)	3948(2)	34(1)
C(33)	1	9376(3)	1983(3)	4140(2)	38(1)
C(34)	1	9395(3)	2240(3)	4951(2)	41(1)
C(35)	1	8346(3)	2630(3)	5534(2)	34(1)
C(36)	1	7618(3)	3391(3)	5215(2)	31(1)
C(37)	1	7067(3)	5033(2)	5175(2)	28(1)
C(38)	1	6319(3)	5482(3)	6010(2)	28(1)
C(39)	1	5611(3)	6503(3)	6035(2)	31(1)
C(310)	1	6155(3)	7048(3)	5709(2)	32(1)
C(311)	1	6854(3)	6610(3)	4857(2)	35(1)
C(312)	1	7591(3)	5611(3)	4843(2)	31(1)

C(313)	1	8814(3)	3243(3)	2494(2)	49(1)
C(314)	1	9134(4)	843(3)	2190(3)	64(1)
O(41)	1	8144(2)	7683(2)	2791(2)	48(1)
O(42)	1	9466(2)	8034(2)	2506(2)	40(1)
O(43)	1	7748(2)	8261(2)	4432(2)	36(1)
O(44)	1	7774(2)	9289(2)	5327(1)	31(1)
O(45)	1	5761(2)	9954(2)	6391(1)	36(1)
O(46)	1	4791(2)	11879(2)	7007(1)	37(1)
N(41)	1	8369(3)	7930(3)	6291(2)	53(1)
N(42)	1	9100(3)	7690(3)	6492(2)	59(1)
N(43)	1	9726(4)	7481(3)	6770(2)	77(1)
N(44)	1	5088(3)	13100(2)	5799(2)	41(1)
N(45)	1	4579(3)	13663(3)	6432(2)	39(1)
N(46)	1	4059(3)	14270(3)	6930(2)	55(1)
N(47)	1	8026(2)	10412(2)	4132(2)	39(1)
N(48)	1	8918(3)	9979(3)	4063(2)	44(1)
N(49)	1	9754(3)	9585(3)	3932(3)	67(1)
C(41)	1	8548(3)	8203(3)	3056(2)	35(1)
C(42)	1	8675(3)	8004(3)	3854(2)	37(1)
C(43)	1	9509(3)	7684(3)	4027(2)	39(1)
C(44)	1	9531(3)	7594(3)	4875(2)	42(1)
C(45)	1	8534(3)	7710(3)	5437(2)	41(1)
C(46)	1	7696(3)	8473(3)	5230(2)	36(1)
C(47)	1	6926(3)	10148(3)	5313(2)	28(1)
C(48)	1	6187(3)	10561(3)	6147(2)	29(1)
C(49)	1	5386(3)	11541(3)	6186(2)	29(1)
C(410)	1	5833(3)	12173(3)	5844(2)	34(1)
C(411)	1	6528(3)	11754(3)	4989(2)	34(1)
C(412)	1	7360(3)	10794(3)	4974(2)	30(1)
C(413)	1	8730(4)	6692(3)	2665(3)	60(1)
C(414)	1	9388(3)	8384(3)	1775(2)	50(1)
O(51)	0.75	2935(3)	2663(2)	6851(2)	33(1)
O(52)	0.75	1894(2)	2037(2)	6789(2)	35(1)
O(53)	0.75	3476(3)	2435(6)	5110(2)	33(1)
C(51)	0.75	2734(3)	2138(2)	6368(2)	28(1)
C(52)	0.75	2583(3)	2516(3)	5615(2)	30(1)
C(53)	0.75	1743(3)	2839(4)	5456(3)	44(2)
C(54)	0.75	1696(3)	3169(5)	4656(3)	50(1)
C(513)	0.75	2168(5)	3611(3)	7113(4)	48(2)
C(514)	0.75	2054(4)	1421(3)	7378(3)	40(1)
O(91)	0.25	2883(10)	3015(7)	6876(8)	33(1)
O(92)	0.25	3005(6)	1632(5)	6436(4)	35(1)
O(93)	0.25	3400(8)	2540(19)	5147(6)	33(1)
C(91)	0.25	2483(7)	2602(4)	6487(3)	28(1)
C(92)	0.25	2448(7)	2840(10)	5676(4)	30(1)
C(93)	0.25	1642(7)	3176(17)	5466(5)	44(2)
C(94)	0.25	1688(5)	3279(12)	4602(4)	50(1)
C(913)	0.25	2182(16)	3938(10)	7295(14)	48(2)
C(914)	0.25	2822(11)	1303(7)	7195(6)	40(1)
O(54)	1	3314(2)	3657(2)	4337(1)	31(1)
O(55)	1	5373(2)	2664(2)	3262(1)	32(1)
O(56)	1	6232(2)	3835(2)	2682(1)	35(1)
N(51)	1	2848(3)	2837(3)	3220(2)	50(1)
N(52)	1	2364(3)	3681(3)	3179(2)	51(1)
N(53)	1	1978(4)	4411(3)	3045(2)	75(1)
N(54)	1	5793(3)	5373(2)	3883(2)	45(1)
N(55)	1	6354(2)	5428(2)	3239(2)	38(1)
N(56)	1	6910(3)	5524(2)	2729(2)	46(1)
N(57)	1	2953(3)	5052(2)	5523(2)	46(1)
N(58)	1	2114(3)	5234(3)	5588(2)	56(1)
N(59)	1	1303(3)	5418(3)	5738(3)	86(2)
C(55)	1	2721(3)	2636(3)	4055(2)	42(1)

C(56)	1	3501(3)	2727(3)	4339(2)	34(1)
C(57)	1	4121(3)	3839(2)	4349(2)	28(1)
C(58)	1	4873(3)	3634(3)	3509(2)	27(1)
C(59)	1	5612(3)	3996(3)	3501(2)	30(1)
C(510)	1	5097(3)	5027(3)	3825(2)	31(1)
C(511)	1	4393(3)	5194(3)	4675(2)	37(1)
C(512)	1	3627(3)	4868(3)	4681(2)	32(1)
O(61)	1	3100(2)	7419(2)	6905(2)	51(1)
O(62)	1	1684(2)	8861(2)	7248(2)	51(1)
O(63)	1	3399(2)	7700(2)	5303(2)	49(1)
O(64)	1	3346(2)	8692(2)	4344(2)	37(1)
O(65)	1	5342(2)	7630(2)	3270(2)	42(1)
O(66)	1	6303(2)	8732(2)	2632(1)	38(1)
N(64)	1	5981(3)	10222(3)	3817(2)	44(1)
N(65)	1	6438(2)	10393(2)	3190(2)	33(1)
N(66)	1	6918(3)	10569(2)	2675(2)	42(1)
N(67)	1	3092(2)	10036(2)	5532(2)	39(1)
N(68)	1	2204(3)	10409(2)	5625(2)	46(1)
N(69)	1	1350(3)	10767(3)	5788(3)	76(1)
C(61)	1	2603(3)	8310(3)	6671(3)	46(1)
C(62)	1	2472(3)	8228(3)	5870(3)	43(1)
C(67)	1	4175(3)	8836(3)	4348(2)	33(1)
C(68)	1	4918(3)	8599(3)	3498(2)	31(1)
C(69)	1	5703(3)	8905(3)	3458(2)	33(1)
C(610)	1	5240(3)	9926(3)	3781(2)	33(1)
C(611)	1	4547(3)	10115(3)	4645(2)	33(1)
C(612)	1	3735(3)	9857(3)	4682(2)	32(1)
C(613)	1	1778(4)	9117(3)	7972(3)	64(1)
C(614)	1	2617(4)	6854(3)	6961(3)	60(1)
O(71)	1	3011(2)	6078(2)	-1013(2)	45(1)
O(72)	1	1452(2)	6155(2)	-426(2)	50(1)
O(73)	1	3443(2)	5515(2)	365(2)	42(1)
O(74)	1	3479(2)	4581(2)	1368(1)	33(1)
O(75)	1	5478(2)	3910(2)	1370(2)	34(1)
O(76)	1	6445(2)	2006(2)	1538(1)	37(1)
N(71)	1	3094(3)	5968(3)	2524(3)	64(1)
N(72)	1	2463(3)	6101(3)	3139(3)	58(1)
N(73)	1	1885(4)	6266(4)	3778(3)	78(1)
N(74)	1	6114(3)	747(2)	566(2)	44(1)
N(75)	1	6644(3)	182(2)	915(2)	38(1)
N(76)	1	7168(3)	-417(3)	1142(2)	49(1)
N(77)	1	3120(3)	3397(3)	484(2)	43(1)
N(78)	1	2250(3)	3882(3)	920(2)	48(1)
N(79)	1	1427(3)	4318(3)	1265(3)	69(1)
C(71)	1	2439(3)	5732(3)	-454(2)	40(1)
C(72)	1	2466(3)	5869(3)	385(2)	37(1)
C(73)	1	1691(3)	6228(3)	1040(3)	45(1)
C(74)	1	1783(3)	6303(3)	1860(3)	50(1)
C(75)	1	2821(3)	6156(3)	1768(3)	52(1)
C(76)	1	3590(3)	5349(3)	1130(2)	38(1)
C(77)	1	4283(2)	3696(3)	963(2)	26(1)
C(78)	1	5039(3)	3313(3)	1400(2)	27(1)
C(79)	1	5838(3)	2311(3)	1039(2)	30(1)
C(710)	1	5369(3)	1679(3)	1000(2)	31(1)
C(711)	1	4653(3)	2073(3)	530(2)	34(1)
C(712)	1	3836(3)	3049(3)	938(2)	32(1)
C(713)	1	2700(4)	7045(3)	-834(3)	63(1)
C(714)	1	1340(4)	5902(4)	-1151(3)	64(1)
O(81)	1	2951(2)	11066(2)	-838(2)	36(1)
O(82)	1	1757(2)	12567(2)	-184(2)	35(1)
O(83)	1	3466(2)	10803(2)	582(1)	31(1)
O(84)	1	3347(2)	9691(2)	1393(1)	29(1)

O(85)	1	5390(2)	8899(2)	1425(2)	31(1)
O(86)	1	6221(2)	6980(2)	1580(1)	32(1)
N(81)	1	2998(2)	10784(2)	2767(2)	44(1)
N(84)	1	5825(3)	5821(2)	584(2)	39(1)
N(85)	1	6360(3)	5285(2)	948(2)	32(1)
N(86)	1	6905(3)	4706(2)	1179(2)	37(1)
N(87)	1	3092(2)	8600(2)	313(2)	44(1)
C(81)	1	2656(3)	11796(3)	-224(2)	31(1)
C(82)	1	2557(3)	11489(3)	592(2)	30(1)
C(83)	1	1745(3)	11858(3)	1230(2)	37(1)
C(84)	1	1751(3)	11563(3)	2037(2)	39(1)
C(85)	1	2803(3)	11199(3)	2044(2)	33(1)
C(86)	1	3545(3)	10453(2)	1320(2)	29(1)
C(87)	1	4159(2)	8809(2)	965(2)	25(1)
C(88)	1	4885(3)	8358(2)	1429(2)	27(1)
C(89)	1	5642(3)	7348(3)	1065(2)	28(1)
C(810)	1	5126(3)	6780(3)	993(2)	31(1)
C(811)	1	4464(3)	7209(3)	485(2)	33(1)
C(812)	1	3680(3)	8211(2)	861(2)	30(1)
C(813)	1	2267(3)	10693(3)	-734(3)	46(1)
C(814)	1	1851(3)	13087(3)	-831(2)	40(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C14 H21 N9 O6.

	Occ.	x	y	z	U_{eq}
H(15)	1	5370	1383	7942	48
H(16)	1	4287	453	8383	46
H(11)	1	7987	2395	9976	36
H(13)	1	9980	1148	8359	39
H(14A)	1	9769	1024	7097	41
H(14B)	1	9600	174	7448	41
H(15A)	1	8080	2036	7630	36
H(16A)	1	6890	1595	8334	30
H(17)	1	6695	389	9164	28
H(18)	1	6620	-13	7605	31
H(19)	1	5124	226	9119	34
H(110)	1	6438	-1467	8003	35
H(11A)	1	7147	-2026	9024	34
H(11B)	1	6425	-1038	9585	34
H(112)	1	7948	-1343	8079	34
H(11C)	1	9057	-39	9739	75
H(11D)	1	8889	-78	10675	75
H(11E)	1	9728	175	10146	75
H(11F)	1	8753	2930	10536	75
H(11G)	1	9942	2450	10263	75
H(11H)	1	9351	1997	10863	75
H(25)	1	5544	6369	7736	56
H(26)	1	4284	5373	8208	52
H(63A)	0.49	1006	8796	6122	54
H(64A)	0.49	1515	9057	4640	74
H(64B)	0.49	1129	8293	4801	74
H(65A)	0.49	2721	7084	4420	85
H(66A)	0.49	4156	7331	4142	61
H(63B)	0.51	1057	9137	6183	54
H(64C)	0.51	1396	9219	4701	74
H(64D)	0.51	959	8503	4968	74
H(65B)	0.51	2497	7228	4494	85
H(66B)	0.51	4007	7325	4101	61
H(21)	1	8119	5273	10134	37
H(23)	1	10109	4994	8594	42
H(24A)	1	9684	4802	7362	47
H(24B)	1	10056	5573	7349	47
H(25A)	1	8491	6768	7720	47
H(26A)	1	7031	6564	8210	38
H(27)	1	6650	5437	9081	32
H(28)	1	6609	4952	7530	35
H(29)	1	5021	5306	9010	33
H(210)	1	6371	3524	8006	36
H(21A)	1	6944	3081	9126	37
H(21B)	1	6236	4122	9592	37
H(212)	1	7862	3621	8112	32
H(21C)	1	9226	5208	11196	75
H(21D)	1	10046	4175	10767	75
H(21E)	1	8891	4486	10941	75
H(21F)	1	9235	6653	10379	79
H(21G)	1	8190	7573	10729	79
H(21H)	1	8626	7168	9795	79

H(35)	1	5413	5173	6732	53
H(36)	1	4407	6999	6904	54
H(31)	1	7889	1930	3347	43
H(33)	1	9968	1519	3759	46
H(34A)	1	9634	2711	4925	50
H(34B)	1	9848	1684	5126	50
H(35A)	1	8161	2113	5580	41
H(36A)	1	6929	3608	5599	37
H(37)	1	6717	4973	4809	33
H(38)	1	6691	5441	6388	34
H(39)	1	5180	6542	5709	38
H(310)	1	6553	7046	6055	38
H(31A)	1	6463	6629	4507	42
H(31B)	1	7217	6970	4648	42
H(312)	1	8009	5601	5172	37
H(31C)	1	8934	3434	2961	73
H(31D)	1	8534	3783	2228	73
H(31E)	1	9444	2767	2118	73
H(31F)	1	8618	673	2481	96
H(31G)	1	9756	277	1925	96
H(31H)	1	8920	1225	1787	96
H(45)	1	5406	10122	6876	54
H(46)	1	4191	12056	7056	56
H(41)	1	8076	8879	3111	42
H(43)	1	10118	7502	3603	47
H(44A)	1	9676	8075	5063	50
H(44B)	1	10068	6976	4884	50
H(45A)	1	8505	7115	5355	49
H(46A)	1	7048	8555	5610	43
H(47)	1	6597	10029	4954	33
H(48)	1	6552	10576	6516	35
H(49)	1	4962	11519	5875	35
H(410)	1	6217	12233	6178	40
H(41A)	1	6818	12166	4764	41
H(41B)	1	6149	11703	4653	41
H(412)	1	7749	10851	5304	36
H(41C)	1	9328	6505	2195	90
H(41D)	1	8340	6400	2574	90
H(41E)	1	8925	6495	3138	90
H(41F)	1	9203	8018	1480	74
H(41G)	1	10030	8337	1450	74
H(41H)	1	8877	9037	1894	74
H(51C)	0.75	3317	1502	6206	34
H(53A)	0.75	1165	2867	5842	53
H(54A)	0.75	1212	3050	4490	60
H(54B)	0.75	1483	3845	4699	60
H(51D)	0.75	2351	3933	7452	71
H(51E)	0.75	1538	3620	7419	71
H(51F)	0.75	2091	3926	6645	71
H(51G)	0.75	1437	1391	7654	60
H(51H)	0.75	2254	1655	7768	60
H(51I)	0.75	2580	798	7113	60
H(91A)	0.25	1783	2802	6839	34
H(93A)	0.25	1014	3360	5866	53
H(94A)	0.25	1202	3124	4480	60
H(94B)	0.25	1517	3930	4518	60
H(91B)	0.25	2519	4198	7523	71
H(91C)	0.25	1643	3913	7726	71
H(91D)	0.25	1905	4333	6920	71
H(91E)	0.25	3220	624	7117	60
H(91F)	0.25	2114	1472	7423	60
H(91G)	0.25	3008	1587	7563	60

H(55)	1	5771	2540	2792	49
H(56)	1	6814	3428	2628	53
H(55A)	1	2882	1965	4032	50
H(56A)	1	4175	2321	3944	40
H(57)	1	4462	3456	4714	33
H(58)	1	4508	3945	3133	33
H(59)	1	6033	3638	3828	36
H(510)	1	4711	5391	3478	38
H(51A)	1	4049	5865	4889	44
H(51B)	1	4778	4850	5023	44
H(512)	1	3225	5237	4345	39
H(65)	1	5749	7477	2802	63
H(66)	1	6867	8279	2561	58
H(61)	1	3023	8631	6626	55
H(67)	1	4513	8437	4707	39
H(68)	1	4549	8926	3129	38
H(69)	1	6130	8527	3774	39
H(610)	1	4852	10309	3442	40
H(61A)	1	4936	9747	4982	39
H(61B)	1	4246	10782	4859	39
H(612)	1	3324	10251	4362	38
H(61C)	1	2138	8555	8184	96
H(61D)	1	1115	9494	8363	96
H(61E)	1	2146	9478	7869	96
H(61F)	1	1931	7198	7325	89
H(61G)	1	2974	6285	7168	89
H(61H)	1	2615	6689	6429	89
H(75)	1	5820	3769	1677	51
H(76)	1	7042	1679	1253	56
H(71)	1	2729	5049	-631	48
H(73)	1	1046	6450	997	53
H(74A)	1	1658	5828	2157	60
H(74B)	1	1284	6925	2168	60
H(75A)	1	2867	6729	1604	63
H(76A)	1	4270	5249	1092	45
H(77)	1	4616	3756	404	32
H(78)	1	4682	3322	1974	32
H(79)	1	6254	2305	486	36
H(710)	1	5006	1631	1554	37
H(71A)	1	4350	1663	500	40
H(71B)	1	5018	2100	-23	40
H(712)	1	3478	3016	1498	38
H(71C)	1	2014	7406	-832	95
H(71D)	1	3138	7220	-1241	95
H(71E)	1	2734	7175	-306	95
H(71F)	1	1723	6083	-1602	96
H(71G)	1	635	6222	-1107	96
H(71H)	1	1585	5228	-1241	96
H(85)	1	5712	8728	1745	47
H(86)	1	6826	6783	1317	48
H(81)	1	3183	12002	-351	37
H(83)	1	1142	12321	1177	44
H(84A)	1	1540	11072	2124	47
H(84B)	1	1289	12100	2468	47
H(85A)	1	2963	11731	2005	39
H(86A)	1	4236	10251	1327	35
H(87)	1	4520	8897	428	30
H(88)	1	4499	8375	1996	32
H(89)	1	6086	7332	523	34
H(810)	1	4712	6765	1538	37
H(81A)	1	4129	6833	437	39
H(81B)	1	4876	7207	-60	39

H(812)	1	3231	8209	1394	36
H(81C)	1	2131	10511	-199	69
H(81D)	1	2557	10147	-1141	69
H(81E)	1	1644	11166	-792	69
H(81F)	1	2359	13279	-848	60
H(81G)	1	1211	13640	-750	60
H(81H)	1	2046	12699	-1337	60

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C14 H21 N9 O6.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(11)	39(2)	39(2)	28(2)	11(1)	-14(1)	-18(1)
O(12)	36(1)	49(2)	34(2)	3(1)	-15(1)	-25(1)
O(13)	29(1)	35(1)	23(1)	4(1)	-10(1)	-17(1)
O(14)	29(1)	25(1)	29(1)	6(1)	-8(1)	-16(1)
O(15)	39(2)	24(1)	39(2)	9(1)	-25(1)	-14(1)
O(16)	31(1)	41(2)	24(1)	6(1)	-13(1)	-18(1)
N(11)	52(2)	35(2)	26(2)	9(1)	-20(2)	-17(2)
N(12)	49(2)	52(2)	38(2)	2(2)	-25(2)	-18(2)
N(13)	63(3)	61(3)	70(3)	-17(2)	-31(2)	-11(2)
N(14)	48(2)	44(2)	30(2)	13(2)	-18(2)	-34(2)
N(15)	35(2)	32(2)	30(2)	6(1)	-10(2)	-17(2)
N(16)	47(2)	43(2)	38(2)	11(2)	-16(2)	-28(2)
N(17)	36(2)	40(2)	42(2)	16(2)	-21(2)	-20(2)
N(18)	39(2)	40(2)	50(2)	5(2)	-19(2)	-15(2)
N(19)	43(3)	100(4)	80(3)	4(3)	-20(2)	-29(2)
C(11)	30(2)	35(2)	29(2)	11(2)	-16(2)	-16(2)
C(12)	34(2)	34(2)	30(2)	10(2)	-16(2)	-19(2)
C(13)	27(2)	38(2)	31(2)	3(2)	-7(2)	-17(2)
C(14)	38(2)	44(2)	21(2)	4(2)	-5(2)	-21(2)
C(15)	42(2)	27(2)	25(2)	8(2)	-13(2)	-19(2)
C(16)	29(2)	26(2)	24(2)	9(2)	-15(2)	-13(2)
C(17)	26(2)	25(2)	22(2)	9(2)	-8(1)	-14(2)
C(18)	34(2)	24(2)	22(2)	2(2)	-11(2)	-15(2)
C(19)	32(2)	34(2)	19(2)	4(2)	-8(2)	-16(2)
C(110)	39(2)	35(2)	20(2)	6(2)	-10(2)	-22(2)
C(111)	39(2)	24(2)	24(2)	7(2)	-11(2)	-16(2)
C(112)	32(2)	29(2)	26(2)	8(2)	-13(2)	-13(2)
C(113)	74(3)	33(3)	49(3)	14(2)	-32(2)	-23(2)
C(114)	65(3)	63(3)	43(3)	6(2)	-28(2)	-40(3)
O(21)	35(2)	37(2)	36(2)	5(1)	-15(1)	-10(1)
O(22)	35(2)	35(2)	36(2)	-1(1)	-10(1)	-13(1)
O(23)	30(1)	32(1)	32(2)	5(1)	-14(1)	-13(1)
O(24)	29(1)	27(1)	30(1)	7(1)	-11(1)	-15(1)
O(25)	48(2)	26(1)	48(2)	12(1)	-32(1)	-16(1)
O(26)	32(1)	50(2)	29(1)	12(1)	-17(1)	-21(1)
N(22A)	52(3)	85(5)	37(3)	15(3)	-25(3)	-38(3)
N(23A)	79(4)	96(5)	42(4)	12(3)	-31(3)	-31(4)
N(32A)	49(3)	53(6)	27(3)	5(3)	-8(2)	-27(4)
N(33A)	67(4)	101(5)	37(3)	-4(3)	-9(3)	-45(4)
C(63A)	38(3)	46(12)	68(4)	16(3)	-20(2)	-33(3)
C(64A)	61(4)	85(10)	69(4)	18(4)	-29(3)	-54(5)
C(65A)	84(5)	70(5)	73(4)	-2(3)	-18(4)	-54(5)
C(66A)	57(3)	38(3)	58(3)	0(2)	-9(2)	-29(2)
N(61A)	110(6)	85(4)	58(3)	-29(3)	-30(3)	-47(4)
N(62A)	91(4)	82(5)	60(4)	-9(3)	-22(3)	-58(4)
N(63A)	112(5)	110(5)	52(4)	0(3)	-20(3)	-63(4)
N(82A)	41(3)	62(6)	28(4)	4(3)	-14(3)	-12(4)
N(83A)	61(4)	117(5)	45(4)	32(3)	-29(3)	-34(4)
N(88A)	37(2)	60(3)	55(2)	19(2)	-25(2)	-26(2)

N(89A)	41(3)	99(5)	86(4)	20(4)	-26(3)	-26(3)
N(22B)	52(3)	85(5)	37(3)	15(3)	-25(3)	-38(3)
N(23B)	79(4)	96(5)	42(4)	12(3)	-31(3)	-31(4)
N(32B)	49(3)	53(6)	27(3)	5(3)	-8(2)	-27(4)
N(33B)	67(4)	101(5)	37(3)	-4(3)	-9(3)	-45(4)
C(63B)	38(3)	46(12)	68(4)	16(3)	-20(2)	-33(3)
C(64B)	61(4)	85(10)	69(4)	18(4)	-29(3)	-54(5)
C(65B)	84(5)	70(5)	73(4)	-2(3)	-18(4)	-54(5)
C(66B)	57(3)	38(3)	58(3)	0(2)	-9(2)	-29(2)
N(61B)	110(6)	85(4)	58(3)	-29(3)	-30(3)	-47(4)
N(62B)	91(4)	82(5)	60(4)	-9(3)	-22(3)	-58(4)
N(63B)	112(5)	110(5)	52(4)	0(3)	-20(3)	-63(4)
N(82B)	41(3)	62(6)	28(4)	4(3)	-14(3)	-12(4)
N(83B)	61(4)	117(5)	45(4)	32(3)	-29(3)	-34(4)
N(88B)	37(2)	60(3)	55(2)	19(2)	-25(2)	-26(2)
N(89B)	41(3)	99(5)	86(4)	20(4)	-26(3)	-26(3)
N(21)	78(3)	49(2)	38(2)	20(2)	-29(2)	-27(2)
N(24)	47(2)	45(2)	23(2)	10(1)	-14(2)	-31(2)
N(25)	40(2)	30(2)	24(2)	4(1)	-7(2)	-16(2)
N(26)	50(2)	53(2)	35(2)	9(2)	-16(2)	-33(2)
N(27)	29(2)	33(2)	26(2)	5(1)	-11(1)	-9(1)
N(28)	36(2)	32(2)	40(2)	8(2)	-16(2)	-15(2)
N(29)	31(2)	46(2)	67(3)	7(2)	-11(2)	-14(2)
C(21)	25(2)	31(2)	37(2)	2(2)	-11(2)	-13(2)
C(22)	26(2)	26(2)	36(2)	5(2)	-10(2)	-14(2)
C(23)	36(2)	40(2)	35(2)	6(2)	-13(2)	-22(2)
C(24)	43(2)	45(2)	34(2)	9(2)	-8(2)	-28(2)
C(25)	53(3)	38(2)	36(2)	14(2)	-17(2)	-29(2)
C(26)	43(2)	28(2)	32(2)	11(2)	-21(2)	-18(2)
C(27)	29(2)	29(2)	23(2)	7(2)	-8(2)	-15(2)
C(28)	35(2)	26(2)	26(2)	5(2)	-14(2)	-13(2)
C(29)	29(2)	32(2)	21(2)	1(2)	-7(2)	-13(2)
C(210)	36(2)	37(2)	20(2)	8(2)	-8(2)	-20(2)
C(211)	38(2)	37(2)	23(2)	9(2)	-13(2)	-20(2)
C(212)	36(2)	24(2)	19(2)	4(2)	-12(2)	-11(2)
C(213)	56(3)	54(3)	42(3)	16(2)	-25(2)	-23(2)
C(214)	76(3)	43(3)	47(3)	3(2)	-21(2)	-35(2)
O(31)	56(2)	47(2)	31(2)	-4(1)	-12(1)	-20(2)
O(32)	40(2)	52(2)	32(2)	15(1)	-16(1)	-23(1)
O(33)	30(1)	36(2)	29(1)	2(1)	-10(1)	-14(1)
O(34)	30(1)	29(1)	34(2)	9(1)	-9(1)	-17(1)
O(35)	41(2)	35(2)	30(2)	1(1)	0(1)	-24(1)
O(36)	39(2)	37(2)	24(1)	5(1)	-7(1)	-13(1)
N(31)	60(2)	55(2)	24(2)	10(2)	-12(2)	-34(2)
N(34)	60(2)	33(2)	27(2)	8(2)	-19(2)	-20(2)
N(35)	47(2)	33(2)	40(2)	17(2)	-24(2)	-25(2)
N(36)	52(2)	42(2)	39(2)	12(2)	-18(2)	-25(2)
N(37)	40(2)	43(2)	29(2)	12(2)	-4(2)	-21(2)
N(38)	44(2)	57(3)	34(2)	7(2)	-8(2)	-29(2)
N(39)	38(2)	85(3)	52(3)	4(2)	-8(2)	-18(2)
C(31)	37(2)	44(3)	30(2)	8(2)	-10(2)	-22(2)
C(32)	38(2)	34(2)	30(2)	6(2)	-10(2)	-18(2)
C(33)	36(2)	42(2)	30(2)	4(2)	-13(2)	-10(2)
C(34)	39(2)	45(3)	35(2)	12(2)	-20(2)	-12(2)
C(35)	50(2)	35(2)	25(2)	13(2)	-16(2)	-26(2)
C(36)	33(2)	32(2)	27(2)	3(2)	-5(2)	-19(2)
C(37)	29(2)	30(2)	27(2)	9(2)	-12(2)	-15(2)
C(38)	32(2)	34(2)	27(2)	11(2)	-14(2)	-20(2)
C(39)	39(2)	36(2)	25(2)	9(2)	-15(2)	-20(2)
C(310)	44(2)	37(2)	24(2)	11(2)	-20(2)	-21(2)
C(311)	48(2)	39(2)	29(2)	12(2)	-18(2)	-26(2)
C(312)	40(2)	37(2)	23(2)	8(2)	-10(2)	-25(2)

C(313)	64(3)	63(3)	33(2)	14(2)	-15(2)	-41(3)
C(314)	99(4)	65(3)	37(3)	-2(2)	-22(3)	-46(3)
O(41)	40(2)	59(2)	43(2)	-4(1)	-14(1)	-22(2)
O(42)	40(2)	48(2)	34(2)	12(1)	-15(1)	-20(1)
O(43)	34(1)	38(2)	33(2)	-3(1)	-7(1)	-17(1)
O(44)	36(1)	30(2)	30(1)	6(1)	-11(1)	-18(1)
O(45)	47(2)	38(2)	26(1)	3(1)	0(1)	-29(1)
O(46)	37(2)	44(2)	24(1)	3(1)	-10(1)	-14(1)
N(41)	66(3)	58(2)	35(2)	18(2)	-15(2)	-30(2)
N(42)	75(3)	61(3)	37(2)	9(2)	-14(2)	-32(2)
N(43)	90(3)	89(3)	47(3)	6(2)	-31(2)	-32(3)
N(44)	60(2)	32(2)	28(2)	10(2)	-22(2)	-15(2)
N(45)	56(2)	33(2)	40(2)	17(2)	-26(2)	-25(2)
N(46)	80(3)	37(2)	43(2)	3(2)	-26(2)	-19(2)
N(47)	31(2)	53(2)	31(2)	12(2)	-7(1)	-20(2)
N(48)	45(3)	48(2)	43(2)	20(2)	-13(2)	-26(2)
N(49)	39(2)	73(3)	78(3)	25(2)	-12(2)	-22(2)
C(41)	24(2)	37(2)	39(2)	-1(2)	-11(2)	-9(2)
C(42)	33(2)	39(2)	31(2)	-2(2)	-3(2)	-14(2)
C(43)	33(2)	40(2)	38(2)	5(2)	-13(2)	-12(2)
C(44)	44(2)	38(2)	35(2)	5(2)	-15(2)	-11(2)
C(45)	52(3)	32(2)	36(2)	1(2)	-14(2)	-18(2)
C(46)	42(2)	37(2)	29(2)	3(2)	-6(2)	-23(2)
C(47)	29(2)	35(2)	21(2)	7(2)	-11(2)	-15(2)
C(48)	35(2)	37(2)	24(2)	9(2)	-12(2)	-23(2)
C(49)	35(2)	38(2)	19(2)	6(2)	-11(2)	-21(2)
C(410)	43(2)	33(2)	30(2)	10(2)	-20(2)	-17(2)
C(411)	48(2)	41(2)	27(2)	12(2)	-19(2)	-27(2)
C(412)	43(2)	41(2)	18(2)	10(2)	-12(2)	-28(2)
C(413)	86(4)	53(3)	49(3)	4(2)	-15(3)	-43(3)
C(414)	58(3)	52(3)	34(2)	13(2)	-16(2)	-22(2)
O(51)	44(2)	25(3)	33(2)	5(2)	-17(1)	-17(2)
O(52)	39(2)	39(2)	26(2)	13(2)	-8(1)	-17(2)
O(53)	30(2)	38(3)	28(2)	12(1)	-6(1)	-16(2)
C(51)	28(3)	19(3)	35(3)	9(3)	-12(2)	-7(3)
C(52)	32(3)	22(4)	31(2)	6(2)	-8(2)	-12(3)
C(53)	36(3)	66(6)	42(3)	29(3)	-16(2)	-30(3)
C(54)	48(3)	83(4)	36(3)	27(2)	-24(2)	-38(3)
C(513)	55(3)	40(5)	32(4)	-5(3)	-11(3)	-10(4)
C(514)	57(3)	36(3)	21(3)	7(2)	-1(2)	-24(3)
O(91)	44(2)	25(3)	33(2)	5(2)	-17(1)	-17(2)
O(92)	39(2)	39(2)	26(2)	13(2)	-8(1)	-17(2)
O(93)	30(2)	38(3)	28(2)	12(1)	-6(1)	-16(2)
C(91)	28(3)	19(3)	35(3)	9(3)	-12(2)	-7(3)
C(92)	32(3)	22(4)	31(2)	6(2)	-8(2)	-12(3)
C(93)	36(3)	66(6)	42(3)	29(3)	-16(2)	-30(3)
C(94)	48(3)	83(4)	36(3)	27(2)	-24(2)	-38(3)
C(913)	55(3)	40(5)	32(4)	-5(3)	-11(3)	-10(4)
C(914)	57(3)	36(3)	21(3)	7(2)	-1(2)	-24(3)
O(54)	39(1)	28(1)	25(1)	3(1)	-9(1)	-16(1)
O(55)	40(2)	27(1)	26(1)	4(1)	-5(1)	-15(1)
O(56)	34(1)	49(2)	29(1)	10(1)	-13(1)	-22(1)
N(51)	75(3)	54(3)	28(2)	3(2)	-16(2)	-37(2)
N(52)	81(3)	58(3)	26(2)	10(2)	-14(2)	-46(2)
N(53)	113(4)	61(3)	52(3)	31(2)	-27(2)	-40(3)
N(54)	69(2)	57(2)	31(2)	14(2)	-23(2)	-44(2)
N(55)	50(2)	42(2)	38(2)	11(2)	-25(2)	-28(2)
N(56)	61(2)	50(2)	41(2)	14(2)	-24(2)	-35(2)
N(57)	51(2)	44(2)	28(2)	-3(2)	0(2)	-17(2)
N(58)	50(3)	42(2)	40(2)	0(2)	9(2)	-8(2)
N(59)	55(3)	88(3)	64(3)	19(2)	11(2)	-9(3)
C(55)	67(3)	49(3)	31(2)	18(2)	-25(2)	-39(2)

C(56)	46(2)	30(2)	24(2)	4(2)	-8(2)	-19(2)
C(57)	36(2)	29(2)	20(2)	8(2)	-13(2)	-15(2)
C(58)	29(2)	26(2)	26(2)	4(2)	-10(2)	-12(2)
C(59)	43(2)	33(2)	22(2)	9(2)	-15(2)	-21(2)
C(510)	50(2)	31(2)	25(2)	13(2)	-23(2)	-22(2)
C(511)	57(3)	32(2)	24(2)	6(2)	-16(2)	-22(2)
C(512)	42(2)	30(2)	20(2)	5(2)	-8(2)	-14(2)
O(61)	41(2)	38(2)	64(2)	19(1)	-12(1)	-13(1)
O(62)	37(2)	52(2)	54(2)	5(2)	-16(1)	-14(1)
O(63)	46(2)	35(2)	62(2)	13(1)	-8(2)	-22(1)
O(64)	44(2)	40(2)	31(2)	0(1)	-10(1)	-24(1)
O(65)	58(2)	33(2)	27(2)	1(1)	-4(1)	-21(1)
O(66)	39(2)	54(2)	23(1)	7(1)	-9(1)	-24(1)
N(64)	66(2)	66(2)	24(2)	18(2)	-23(2)	-45(2)
N(65)	46(2)	29(2)	26(2)	5(2)	-17(2)	-16(2)
N(66)	49(2)	42(2)	35(2)	10(2)	-15(2)	-20(2)
N(67)	32(2)	45(2)	29(2)	-12(2)	-2(1)	-13(2)
N(68)	39(2)	37(2)	54(2)	8(2)	-6(2)	-16(2)
N(69)	44(3)	80(3)	84(3)	36(2)	-9(2)	-22(2)
C(61)	33(2)	33(2)	70(3)	20(2)	-15(2)	-15(2)
C(62)	32(2)	43(3)	51(3)	13(2)	-8(2)	-20(2)
C(67)	38(2)	37(2)	25(2)	6(2)	-12(2)	-18(2)
C(68)	35(2)	29(2)	28(2)	1(2)	-13(2)	-12(2)
C(69)	41(2)	36(2)	21(2)	9(2)	-16(2)	-15(2)
C(610)	45(2)	35(2)	30(2)	8(2)	-22(2)	-22(2)
C(611)	43(2)	33(2)	29(2)	3(2)	-19(2)	-19(2)
C(612)	38(2)	31(2)	25(2)	4(2)	-13(2)	-13(2)
C(613)	72(3)	56(3)	60(3)	6(3)	-31(3)	-20(3)
C(614)	77(3)	38(3)	61(3)	14(2)	-9(3)	-33(2)
O(71)	40(2)	47(2)	47(2)	15(1)	-9(1)	-24(1)
O(72)	37(2)	63(2)	48(2)	3(2)	-12(1)	-24(2)
O(73)	25(2)	37(2)	51(2)	12(1)	-6(1)	-9(1)
O(74)	27(1)	37(2)	29(1)	1(1)	-7(1)	-13(1)
O(75)	38(2)	42(2)	39(2)	16(1)	-21(1)	-28(1)
O(76)	33(2)	45(2)	27(1)	8(1)	-13(1)	-11(1)
N(71)	37(2)	78(3)	54(3)	-31(2)	-16(2)	-7(2)
N(72)	57(3)	59(3)	61(3)	-4(2)	-30(2)	-23(2)
N(73)	84(3)	105(4)	69(3)	31(3)	-46(3)	-50(3)
N(74)	66(2)	33(2)	27(2)	4(2)	-20(2)	-15(2)
N(75)	55(2)	36(2)	25(2)	3(2)	-10(2)	-25(2)
N(76)	66(2)	38(2)	37(2)	8(2)	-21(2)	-16(2)
N(77)	35(2)	57(2)	44(2)	1(2)	-18(2)	-23(2)
N(78)	43(2)	58(2)	54(2)	-1(2)	-23(2)	-28(2)
N(79)	41(2)	76(3)	89(3)	0(2)	-23(2)	-24(2)
C(71)	23(2)	35(2)	52(3)	6(2)	-2(2)	-12(2)
C(72)	26(2)	30(2)	45(3)	7(2)	-6(2)	-9(2)
C(73)	30(2)	44(3)	50(3)	5(2)	-12(2)	-10(2)
C(74)	30(2)	48(3)	53(3)	-6(2)	-8(2)	-6(2)
C(75)	35(2)	39(3)	68(3)	-7(2)	-9(2)	-9(2)
C(76)	29(2)	33(2)	47(3)	1(2)	-12(2)	-10(2)
C(77)	26(2)	35(2)	17(2)	-1(2)	-8(2)	-13(2)
C(78)	31(2)	38(2)	20(2)	8(2)	-12(2)	-20(2)
C(79)	33(2)	41(2)	18(2)	8(2)	-10(2)	-19(2)
C(710)	39(2)	38(2)	18(2)	9(2)	-8(2)	-21(2)
C(711)	40(2)	44(2)	26(2)	7(2)	-13(2)	-26(2)
C(712)	31(2)	43(2)	24(2)	8(2)	-10(2)	-19(2)
C(713)	81(4)	56(3)	78(4)	30(3)	-38(3)	-45(3)
C(714)	63(3)	88(4)	61(3)	12(3)	-23(2)	-50(3)
O(81)	40(2)	40(2)	32(2)	1(1)	-16(1)	-19(1)
O(82)	33(1)	36(2)	33(2)	11(1)	-14(1)	-11(1)
O(83)	28(1)	29(1)	32(2)	8(1)	-14(1)	-8(1)
O(84)	29(1)	27(1)	35(2)	6(1)	-13(1)	-14(1)

O(85)	38(2)	30(1)	38(2)	12(1)	-23(1)	-19(1)
O(86)	32(1)	35(2)	26(1)	3(1)	-13(1)	-11(1)
N(81)	62(2)	53(2)	36(2)	17(2)	-32(2)	-33(2)
N(84)	51(2)	36(2)	25(2)	7(2)	-14(2)	-17(2)
N(85)	45(2)	30(2)	26(2)	3(2)	-10(2)	-23(2)
N(86)	47(2)	31(2)	35(2)	6(2)	-12(2)	-19(2)
N(87)	40(2)	53(2)	48(2)	12(2)	-26(2)	-23(2)
C(81)	33(2)	33(2)	25(2)	2(2)	-10(2)	-14(2)
C(82)	28(2)	27(2)	32(2)	-1(2)	-10(2)	-10(2)
C(83)	26(2)	41(2)	35(2)	7(2)	-12(2)	-7(2)
C(84)	35(2)	45(3)	27(2)	6(2)	-8(2)	-12(2)
C(85)	47(2)	28(2)	30(2)	11(2)	-20(2)	-20(2)
C(86)	32(2)	27(2)	33(2)	9(2)	-16(2)	-14(2)
C(87)	27(2)	24(2)	23(2)	3(2)	-10(2)	-10(2)
C(88)	30(2)	32(2)	23(2)	5(2)	-12(2)	-17(2)
C(89)	36(2)	33(2)	16(2)	4(2)	-9(2)	-16(2)
C(810)	41(2)	32(2)	23(2)	6(2)	-9(2)	-21(2)
C(811)	44(2)	35(2)	31(2)	9(2)	-18(2)	-24(2)
C(812)	35(2)	36(2)	26(2)	8(2)	-15(2)	-20(2)
C(813)	61(3)	42(3)	44(3)	4(2)	-22(2)	-28(2)
C(814)	47(2)	41(2)	28(2)	13(2)	-17(2)	-14(2)

Table 5. Bond lengths [Å] and angles [°] for C14 H21 N9 O6

O(11)-C(11)	1.419(4)	N(22b)-N(23b)	1.138(2)
O(11)-C(113)	1.435(5)	N(22b)-N(21)	1.202(2)
O(12)-C(11)	1.399(4)	N(32b)-N(33b)	1.138(2)
O(12)-C(114)	1.426(4)	N(32b)-N(31)	1.202(2)
O(13)-C(12)	1.374(4)	C(63b)-C(62)	1.311(8)
O(13)-C(16)	1.448(4)	C(63b)-C(64b)	1.527(8)
O(14)-C(16)	1.404(4)	C(64b)-C(65b)	1.536(9)
O(14)-C(17)	1.444(4)	C(65b)-C(66b)	1.500(8)
O(15)-C(18)	1.418(4)	C(65b)-N(61b)	1.541(10)
O(16)-C(19)	1.429(4)	C(66b)-O(64)	1.394(7)
N(11)-N(12)	1.234(4)	C(66b)-O(63)	1.456(6)
N(11)-C(15)	1.494(4)	N(61b)-N(62b)	1.202(2)
N(12)-N(13)	1.130(5)	N(62b)-N(63b)	1.138(2)
N(14)-N(15)	1.204(2)	N(82b)-N(83b)	1.138(2)
N(14)-C(110)	1.493(4)	N(82b)-N(81)	1.201(2)
N(15)-N(16)	1.138(2)	N(88b)-N(89b)	1.138(2)
N(17)-N(18)	1.230(4)	N(88b)-N(87)	1.202(2)
N(17)-C(112)	1.485(4)	N(21)-C(25)	1.468(5)
N(18)-N(19)	1.133(5)	N(24)-N(25)	1.235(4)
C(11)-C(12)	1.514(5)	N(24)-C(210)	1.483(4)
C(12)-C(13)	1.317(4)	N(25)-N(26)	1.141(4)
C(13)-C(14)	1.510(5)	N(27)-N(28)	1.241(4)
C(14)-C(15)	1.499(5)	N(27)-C(212)	1.484(4)
C(15)-C(16)	1.531(5)	N(28)-N(29)	1.137(4)
C(17)-C(112)	1.520(5)	C(21)-C(22)	1.509(5)
C(17)-C(18)	1.521(5)	C(22)-C(23)	1.319(5)
C(18)-C(19)	1.539(5)	C(23)-C(24)	1.508(5)
C(19)-C(110)	1.515(5)	C(24)-C(25)	1.514(6)
C(110)-C(111)	1.518(5)	C(25)-C(26)	1.526(5)
C(111)-C(112)	1.525(5)	C(27)-C(28)	1.523(5)
O(21)-C(21)	1.385(4)	C(27)-C(212)	1.525(5)
O(21)-C(213)	1.441(4)	C(28)-C(29)	1.529(5)
O(22)-C(21)	1.420(4)	C(29)-C(210)	1.521(5)
O(22)-C(214)	1.428(5)	C(210)-C(211)	1.523(5)
O(23)-C(22)	1.386(4)	C(211)-C(212)	1.524(5)
O(23)-C(26)	1.436(4)	O(31)-C(31)	1.373(4)
O(24)-C(26)	1.401(4)	O(31)-C(314)	1.438(5)
O(24)-C(27)	1.436(4)	O(32)-C(31)	1.417(4)
O(25)-C(28)	1.419(4)	O(32)-C(313)	1.430(4)
O(26)-C(29)	1.436(4)	O(33)-C(32)	1.382(4)
N(22a)-N(23a)	1.138(2)	O(33)-C(36)	1.430(4)
N(22a)-N(21)	1.203(2)	O(34)-C(36)	1.401(4)
N(32a)-N(33a)	1.138(2)	O(34)-C(37)	1.441(4)
N(32a)-N(31)	1.202(2)	O(35)-C(38)	1.415(4)
C(63a)-C(62)	1.337(9)	O(36)-C(39)	1.434(4)
C(63a)-C(64a)	1.526(9)	N(31)-C(35)	1.480(4)
C(64a)-C(65a)	1.527(9)	N(34)-N(35)	1.254(4)
C(65a)-N(61a)	1.476(11)	N(34)-C(310)	1.478(5)
C(65a)-C(66a)	1.532(8)	N(35)-N(36)	1.141(4)
C(66a)-O(64)	1.387(7)	N(37)-N(38)	1.244(5)
C(66a)-O(63)	1.403(6)	N(37)-C(312)	1.488(4)
N(61a)-N(62a)	1.203(2)	N(38)-N(39)	1.124(5)
N(62a)-N(63a)	1.139(2)	C(31)-C(32)	1.505(5)
N(82a)-N(83a)	1.138(2)	C(32)-C(33)	1.322(5)
N(82a)-N(81)	1.202(2)	C(33)-C(34)	1.505(5)
N(88a)-N(89a)	1.138(2)	C(34)-C(35)	1.513(5)
N(88a)-N(87)	1.202(2)	C(35)-C(36)	1.513(5)

C(37)-C(312)	1.522(4)	N(52)-N(53)	1.127(5)
C(37)-C(38)	1.523(5)	N(54)-N(55)	1.251(5)
C(38)-C(39)	1.524(5)	N(54)-C(510)	1.474(5)
C(39)-C(310)	1.498(5)	N(55)-N(56)	1.125(4)
C(310)-C(311)	1.523(5)	N(57)-N(58)	1.200(5)
C(311)-C(312)	1.515(5)	N(57)-C(512)	1.490(5)
O(41)-C(41)	1.418(4)	N(58)-N(59)	1.129(5)
O(41)-C(413)	1.431(5)	C(55)-C(56)	1.531(5)
O(42)-C(41)	1.397(4)	C(57)-C(512)	1.522(5)
O(42)-C(414)	1.424(4)	C(57)-C(58)	1.530(5)
O(43)-C(42)	1.397(4)	C(58)-C(59)	1.527(5)
O(43)-C(46)	1.422(4)	C(59)-C(510)	1.519(5)
O(44)-C(46)	1.399(4)	C(510)-C(511)	1.522(5)
O(44)-C(47)	1.451(4)	C(511)-C(512)	1.526(5)
O(45)-C(48)	1.427(4)	O(61)-C(614)	1.422(5)
O(46)-C(49)	1.424(4)	O(61)-C(61)	1.434(5)
N(41)-N(42)	1.213(5)	O(62)-C(61)	1.390(5)
N(41)-C(45)	1.469(5)	O(62)-C(613)	1.416(5)
N(42)-N(43)	1.154(5)	O(63)-C(62)	1.384(5)
N(44)-N(45)	1.247(5)	O(64)-C(67)	1.440(4)
N(44)-C(410)	1.463(5)	O(65)-C(68)	1.411(4)
N(45)-N(46)	1.130(4)	O(66)-C(69)	1.434(4)
N(47)-N(48)	1.237(5)	N(64)-N(65)	1.237(4)
N(47)-C(412)	1.485(4)	N(64)-C(610)	1.472(5)
N(48)-N(49)	1.135(5)	N(65)-N(66)	1.128(4)
C(41)-C(42)	1.497(5)	N(67)-N(68)	1.220(5)
C(42)-C(43)	1.321(5)	N(67)-C(612)	1.488(4)
C(43)-C(44)	1.515(5)	N(68)-N(69)	1.153(5)
C(44)-C(45)	1.528(5)	C(61)-C(62)	1.506(6)
C(45)-C(46)	1.502(5)	C(67)-C(612)	1.521(5)
C(47)-C(48)	1.509(5)	C(67)-C(68)	1.531(5)
C(47)-C(412)	1.527(5)	C(68)-C(69)	1.519(5)
C(48)-C(49)	1.516(5)	C(69)-C(610)	1.512(5)
C(49)-C(410)	1.521(5)	C(610)-C(611)	1.531(5)
C(410)-C(411)	1.521(5)	C(611)-C(612)	1.510(5)
C(411)-C(412)	1.523(5)	O(71)-C(713)	1.425(5)
O(51)-C(51)	1.403(3)	O(71)-C(71)	1.426(4)
O(51)-C(513)	1.438(4)	O(72)-C(71)	1.390(4)
O(52)-C(51)	1.403(3)	O(72)-C(714)	1.430(5)
O(52)-C(514)	1.438(4)	O(73)-C(72)	1.383(4)
O(53)-C(52)	1.383(4)	O(73)-C(76)	1.443(5)
O(53)-C(56)	1.435(4)	O(74)-C(76)	1.382(4)
C(51)-C(52)	1.503(5)	O(74)-C(77)	1.428(4)
C(52)-C(53)	1.316(4)	O(75)-C(78)	1.419(4)
C(53)-C(54)	1.519(5)	O(76)-C(79)	1.425(4)
C(54)-C(55)	1.502(6)	N(71)-N(72)	1.182(6)
O(91)-C(91)	1.403(3)	N(71)-C(75)	1.512(6)
O(91)-C(913)	1.438(4)	N(72)-N(73)	1.165(5)
O(92)-C(91)	1.403(3)	N(74)-N(75)	1.243(5)
O(92)-C(914)	1.438(4)	N(74)-C(710)	1.468(5)
O(93)-C(92)	1.383(4)	N(75)-N(76)	1.130(4)
O(93)-C(56)	1.435(4)	N(77)-N(78)	1.236(5)
C(91)-C(92)	1.493(8)	N(77)-C(712)	1.491(5)
C(92)-C(93)	1.317(4)	N(78)-N(79)	1.134(5)
C(93)-C(94)	1.519(6)	C(71)-C(72)	1.517(5)
C(94)-C(55)	1.502(6)	C(72)-C(73)	1.310(5)
O(54)-C(56)	1.402(4)	C(73)-C(74)	1.510(6)
O(54)-C(57)	1.445(4)	C(74)-C(75)	1.515(6)
O(55)-C(58)	1.409(4)	C(75)-C(76)	1.500(5)
O(56)-C(59)	1.436(4)	C(77)-C(712)	1.513(5)
N(51)-N(52)	1.252(5)	C(77)-C(78)	1.519(5)
N(51)-C(55)	1.483(5)	C(78)-C(79)	1.534(5)

C(79)-C(710)	1.526(5)
C(710)-C(711)	1.516(5)
C(711)-C(712)	1.528(5)
O(81)-C(81)	1.419(4)
O(81)-C(813)	1.432(4)
O(82)-C(81)	1.401(4)
O(82)-C(814)	1.429(4)
O(83)-C(82)	1.371(4)
O(83)-C(86)	1.438(4)
O(84)-C(86)	1.403(4)
O(84)-C(87)	1.439(4)
O(85)-C(88)	1.427(4)
O(86)-C(89)	1.426(4)
N(81)-C(85)	1.491(4)
N(84)-N(85)	1.246(4)
N(84)-C(810)	1.473(5)
N(85)-N(86)	1.132(4)
N(87)-C(812)	1.490(4)
C(81)-C(82)	1.511(5)
C(82)-C(83)	1.322(5)
C(83)-C(84)	1.504(5)
C(84)-C(85)	1.508(5)
C(85)-C(86)	1.531(5)
C(87)-C(812)	1.516(4)
C(87)-C(88)	1.531(5)
C(88)-C(89)	1.531(5)
C(89)-C(810)	1.509(5)
C(810)-C(811)	1.515(5)
C(811)-C(812)	1.533(5)

C(11)-O(11)-C(113)	114.4(3)
C(11)-O(12)-C(114)	113.8(3)
C(12)-O(13)-C(16)	118.3(2)
C(16)-O(14)-C(17)	115.8(2)
N(12)-N(11)-C(15)	113.5(3)
N(13)-N(12)-N(11)	173.5(4)
N(15)-N(14)-C(110)	118.0(3)
N(16)-N(15)-N(14)	170.4(3)
N(18)-N(17)-C(112)	115.6(3)
N(19)-N(18)-N(17)	173.1(4)
O(12)-C(11)-O(11)	112.1(3)
O(12)-C(11)-C(12)	107.8(3)
O(11)-C(11)-C(12)	113.5(3)
C(13)-C(12)-O(13)	125.7(3)
C(13)-C(12)-C(11)	125.4(3)
O(13)-C(12)-C(11)	108.9(3)
C(12)-C(13)-C(14)	120.3(3)
C(15)-C(14)-C(13)	107.6(3)
N(11)-C(15)-C(14)	115.1(3)
N(11)-C(15)-C(16)	108.1(3)
C(14)-C(15)-C(16)	111.8(3)
O(14)-C(16)-O(13)	110.6(3)
O(14)-C(16)-C(15)	107.4(3)
O(13)-C(16)-C(15)	111.5(3)
O(14)-C(17)-C(112)	105.0(3)
O(14)-C(17)-C(18)	111.6(3)
C(112)-C(17)-C(18)	110.9(3)
O(15)-C(18)-C(17)	109.2(3)
O(15)-C(18)-C(19)	109.5(3)
C(17)-C(18)-C(19)	111.4(3)
O(16)-C(19)-C(110)	110.6(3)
O(16)-C(19)-C(18)	107.5(3)
C(110)-C(19)-C(18)	110.8(3)
N(14)-C(110)-C(19)	111.5(3)
N(14)-C(110)-C(111)	107.2(3)
C(19)-C(110)-C(111)	110.0(3)
C(110)-C(111)-C(112)	110.4(3)
N(17)-C(112)-C(17)	110.3(3)
N(17)-C(112)-C(111)	107.1(3)
C(17)-C(112)-C(111)	111.1(3)
C(21)-O(21)-C(213)	112.1(3)
C(21)-O(22)-C(214)	115.4(3)
C(22)-O(23)-C(26)	114.3(3)
C(26)-O(24)-C(27)	115.6(3)
N(23A)-N(22A)-N(21)	170.8(7)
N(33A)-N(32A)-N(31)	171.5(7)
C(62)-C(63A)-C(64A)	120.3(8)
C(63A)-C(64A)-C(65A)	110.9(6)
N(61A)-C(65A)-C(64A)	118.0(8)
N(61A)-C(65A)-C(66A)	106.3(8)
C(64A)-C(65A)-C(66A)	109.2(7)
O(64)-C(66A)-O(63)	113.0(5)
O(64)-C(66A)-C(65A)	104.6(10)
O(63)-C(66A)-C(65A)	109.7(5)
N(62A)-N(61A)-C(65A)	119.8(7)
N(63A)-N(62A)-N(61A)	169.9(7)
N(83A)-N(82A)-N(81)	172.3(7)
N(89A)-N(88A)-N(87)	172.2(7)
N(23B)-N(22B)-N(21)	171.1(7)
N(33B)-N(32B)-N(31)	172.2(7)
C(62)-C(63B)-C(64B)	120.7(6)
C(63B)-C(64B)-C(65B)	109.0(6)
C(66B)-C(65B)-C(64B)	111.3(7)
C(66B)-C(65B)-N(61B)	107.9(7)
C(64B)-C(65B)-N(61B)	112.2(7)
O(64)-C(66B)-O(63)	109.4(5)
O(64)-C(66B)-C(65B)	107.4(10)
O(63)-C(66B)-C(65B)	111.7(5)
N(62B)-N(61B)-C(65B)	120.1(7)
N(63B)-N(62B)-N(61B)	172.5(8)
N(83B)-N(82B)-N(81)	172.0(7)
N(89B)-N(88B)-N(87)	172.2(7)
N(22B)-N(21)-N(22A)	32.4(5)
N(22B)-N(21)-C(25)	122.0(4)
N(22A)-N(21)-C(25)	114.2(5)
N(25)-N(24)-C(210)	118.4(3)
N(26)-N(25)-N(24)	169.3(3)
N(28)-N(27)-C(212)	114.1(3)
N(29)-N(28)-N(27)	173.5(4)
O(21)-C(21)-O(22)	112.3(3)
O(21)-C(21)-C(22)	108.5(3)
O(22)-C(21)-C(22)	113.0(3)
C(23)-C(22)-O(23)	123.9(3)
C(23)-C(22)-C(21)	126.5(3)
O(23)-C(22)-C(21)	109.4(3)
C(22)-C(23)-C(24)	122.5(4)
C(23)-C(24)-C(25)	110.7(3)
N(21)-C(25)-C(24)	115.9(3)
N(21)-C(25)-C(26)	107.3(3)
C(24)-C(25)-C(26)	110.2(3)
O(24)-C(26)-O(23)	110.7(3)
O(24)-C(26)-C(25)	106.3(3)
O(23)-C(26)-C(25)	110.3(3)
O(24)-C(27)-C(28)	110.1(3)

O(24)-C(27)-C(212)	105.7(3)	N(45)-N(44)-C(410)	117.9(3)
C(28)-C(27)-C(212)	111.6(3)	N(46)-N(45)-N(44)	169.2(4)
O(25)-C(28)-C(27)	106.8(3)	N(48)-N(47)-C(412)	113.6(3)
O(25)-C(28)-C(29)	110.8(3)	N(49)-N(48)-N(47)	174.2(4)
C(27)-C(28)-C(29)	112.5(3)	O(42)-C(41)-O(41)	111.7(3)
O(26)-C(29)-C(210)	109.8(3)	O(42)-C(41)-C(42)	108.7(3)
O(26)-C(29)-C(28)	106.9(3)	O(41)-C(41)-C(42)	112.2(3)
C(210)-C(29)-C(28)	110.9(3)	C(43)-C(42)-O(43)	123.0(3)
N(24)-C(210)-C(29)	112.7(3)	C(43)-C(42)-C(41)	127.2(3)
N(24)-C(210)-C(211)	105.4(3)	O(43)-C(42)-C(41)	109.7(3)
C(29)-C(210)-C(211)	109.4(3)	C(42)-C(43)-C(44)	122.5(3)
C(210)-C(211)-C(212)	110.1(3)	C(43)-C(44)-C(45)	110.6(3)
N(27)-C(212)-C(211)	108.6(3)	N(41)-C(45)-C(46)	107.8(3)
N(27)-C(212)-C(27)	109.8(3)	N(41)-C(45)-C(44)	114.3(3)
C(211)-C(212)-C(27)	110.2(3)	C(46)-C(45)-C(44)	109.9(3)
C(31)-O(31)-C(314)	112.6(3)	O(44)-C(46)-O(43)	111.0(3)
C(31)-O(32)-C(313)	114.5(3)	O(44)-C(46)-C(45)	107.0(3)
C(32)-O(33)-C(36)	117.6(3)	O(43)-C(46)-C(45)	111.1(3)
C(36)-O(34)-C(37)	116.4(2)	O(44)-C(47)-C(48)	110.8(3)
N(32B)-N(31)-N(32A)	32.4(5)	O(44)-C(47)-C(412)	105.1(3)
N(32B)-N(31)-C(35)	114.7(4)	C(48)-C(47)-C(412)	110.8(3)
N(32A)-N(31)-C(35)	118.8(4)	O(45)-C(48)-C(47)	107.0(3)
N(35)-N(34)-C(310)	116.8(3)	O(45)-C(48)-C(49)	110.8(3)
N(36)-N(35)-N(34)	170.7(4)	C(47)-C(48)-C(49)	112.7(3)
N(38)-N(37)-C(312)	115.6(3)	O(46)-C(49)-C(48)	107.3(3)
N(39)-N(38)-N(37)	172.3(4)	O(46)-C(49)-C(410)	110.6(3)
O(31)-C(31)-O(32)	112.3(3)	C(48)-C(49)-C(410)	111.5(3)
O(31)-C(31)-C(32)	108.8(3)	N(44)-C(410)-C(411)	106.1(3)
O(32)-C(31)-C(32)	112.8(3)	N(44)-C(410)-C(49)	113.2(3)
C(33)-C(32)-O(33)	124.6(3)	C(411)-C(410)-C(49)	109.4(3)
C(33)-C(32)-C(31)	125.9(3)	C(410)-C(411)-C(412)	110.3(3)
O(33)-C(32)-C(31)	109.4(3)	N(47)-C(412)-C(411)	108.7(3)
C(32)-C(33)-C(34)	121.5(3)	N(47)-C(412)-C(47)	110.1(3)
C(33)-C(34)-C(35)	107.8(3)	C(411)-C(412)-C(47)	110.3(3)
N(31)-C(35)-C(34)	115.6(3)	C(51)-O(51)-C(513)	113.8(2)
N(31)-C(35)-C(36)	108.4(3)	C(51)-O(52)-C(514)	113.8(2)
C(34)-C(35)-C(36)	110.8(3)	C(52)-O(53)-C(56)	117.7(3)
O(34)-C(36)-O(33)	110.6(3)	O(52)-C(51)-O(51)	111.7(4)
O(34)-C(36)-C(35)	107.3(3)	O(52)-C(51)-C(52)	107.7(2)
O(33)-C(36)-C(35)	112.3(3)	O(51)-C(51)-C(52)	114.8(3)
O(34)-C(37)-C(312)	105.3(3)	C(53)-C(52)-O(53)	126.0(4)
O(34)-C(37)-C(38)	111.9(3)	C(53)-C(52)-C(51)	125.2(4)
C(312)-C(37)-C(38)	110.8(3)	O(53)-C(52)-C(51)	108.8(3)
O(35)-C(38)-C(37)	108.3(3)	C(52)-C(53)-C(54)	120.1(4)
O(35)-C(38)-C(39)	110.5(3)	C(55)-C(54)-C(53)	107.3(4)
C(37)-C(38)-C(39)	112.0(3)	C(91)-O(91)-C(913)	113.8(2)
O(36)-C(39)-C(310)	110.3(3)	C(91)-O(92)-C(914)	113.8(2)
O(36)-C(39)-C(38)	107.8(3)	C(92)-O(93)-C(56)	117.5(6)
C(310)-C(39)-C(38)	112.2(3)	O(92)-C(91)-O(91)	109.0(7)
N(34)-C(310)-C(39)	113.2(3)	O(92)-C(91)-C(92)	109.1(6)
N(34)-C(310)-C(311)	106.0(3)	O(91)-C(91)-C(92)	117.1(7)
C(39)-C(310)-C(311)	110.1(3)	C(93)-C(92)-O(93)	124.2(6)
C(312)-C(311)-C(310)	110.2(3)	C(93)-C(92)-C(91)	125.0(6)
N(37)-C(312)-C(311)	107.2(3)	O(93)-C(92)-C(91)	110.2(5)
N(37)-C(312)-C(37)	110.6(3)	C(92)-C(93)-C(94)	121.9(6)
C(311)-C(312)-C(37)	111.6(3)	C(55)-C(94)-C(93)	109.2(6)
C(41)-O(41)-C(413)	116.0(3)	C(56)-O(54)-C(57)	115.9(3)
C(41)-O(42)-C(414)	113.1(3)	N(52)-N(51)-C(55)	113.2(3)
C(42)-O(43)-C(46)	114.6(3)	N(53)-N(52)-N(51)	171.7(4)
C(46)-O(44)-C(47)	115.9(3)	N(55)-N(54)-C(510)	117.0(3)
N(42)-N(41)-C(45)	117.2(4)	N(56)-N(55)-N(54)	170.0(4)
N(43)-N(42)-N(41)	172.4(5)	N(58)-N(57)-C(512)	114.7(3)

N(59)-N(58)-N(57)	172.4(5)	C(612)-C(611)-C(610)	110.7(3)
N(51)-C(55)-C(94)	110.8(5)	N(67)-C(612)-C(611)	108.8(3)
N(51)-C(55)-C(54)	116.7(4)	N(67)-C(612)-C(67)	109.6(3)
C(94)-C(55)-C(54)	7.6(9)	C(611)-C(612)-C(67)	110.8(3)
N(51)-C(55)-C(56)	109.6(3)	C(713)-O(71)-C(71)	114.9(3)
C(94)-C(55)-C(56)	110.7(6)	C(71)-O(72)-C(714)	112.3(3)
C(54)-C(55)-C(56)	111.4(4)	C(72)-O(73)-C(76)	114.9(3)
O(54)-C(56)-O(53)	112.9(4)	C(76)-O(74)-C(77)	116.0(3)
O(54)-C(56)-O(93)	107.3(12)	N(72)-N(71)-C(75)	119.2(4)
O(53)-C(56)-O(93)	6.3(14)	N(73)-N(72)-N(71)	173.7(5)
O(54)-C(56)-C(55)	106.8(3)	N(75)-N(74)-C(710)	118.9(3)
O(53)-C(56)-C(55)	111.2(3)	N(76)-N(75)-N(74)	170.6(4)
O(93)-C(56)-C(55)	111.3(6)	N(78)-N(77)-C(712)	113.1(3)
O(54)-C(57)-C(512)	105.0(3)	N(79)-N(78)-N(77)	174.1(4)
O(54)-C(57)-C(58)	111.6(3)	O(72)-C(71)-O(71)	111.8(3)
C(512)-C(57)-C(58)	110.6(3)	O(72)-C(71)-C(72)	108.5(3)
O(55)-C(58)-C(59)	110.7(3)	O(71)-C(71)-C(72)	112.0(3)
O(55)-C(58)-C(57)	108.2(3)	C(73)-C(72)-O(73)	124.5(4)
C(59)-C(58)-C(57)	111.2(3)	C(73)-C(72)-C(71)	125.7(4)
O(56)-C(59)-C(510)	109.7(3)	O(73)-C(72)-C(71)	109.7(3)
O(56)-C(59)-C(58)	106.8(3)	C(72)-C(73)-C(74)	122.5(4)
C(510)-C(59)-C(58)	112.3(3)	C(73)-C(74)-C(75)	109.2(3)
N(54)-C(510)-C(59)	113.1(3)	C(76)-C(75)-N(71)	106.9(3)
N(54)-C(510)-C(511)	106.0(3)	C(76)-C(75)-C(74)	110.9(3)
C(59)-C(510)-C(511)	109.0(3)	N(71)-C(75)-C(74)	114.0(4)
C(510)-C(511)-C(512)	110.3(3)	O(74)-C(76)-O(73)	110.7(3)
N(57)-C(512)-C(57)	110.4(3)	O(74)-C(76)-C(75)	106.3(3)
N(57)-C(512)-C(511)	108.1(3)	O(73)-C(76)-C(75)	110.7(3)
C(57)-C(512)-C(511)	111.7(3)	O(74)-C(77)-C(712)	106.8(3)
C(614)-O(61)-C(61)	114.9(3)	O(74)-C(77)-C(78)	111.3(3)
C(61)-O(62)-C(613)	112.2(3)	C(712)-C(77)-C(78)	109.9(3)
C(62)-O(63)-C(66A)	117.0(5)	O(75)-C(78)-C(77)	107.9(3)
C(62)-O(63)-C(66B)	112.0(4)	O(75)-C(78)-C(79)	110.6(3)
C(66A)-O(63)-C(66B)	5.8(6)	C(77)-C(78)-C(79)	112.2(3)
C(66A)-O(64)-C(66B)	6.3(6)	O(76)-C(79)-C(710)	110.7(3)
C(66A)-O(64)-C(67)	111.9(4)	O(76)-C(79)-C(78)	106.8(3)
C(66B)-O(64)-C(67)	118.2(4)	C(710)-C(79)-C(78)	111.1(3)
N(65)-N(64)-C(610)	117.7(3)	N(74)-C(710)-C(711)	105.8(3)
N(66)-N(65)-N(64)	171.4(4)	N(74)-C(710)-C(79)	111.8(3)
N(68)-N(67)-C(612)	113.8(3)	C(711)-C(710)-C(79)	109.4(3)
N(69)-N(68)-N(67)	173.6(4)	C(710)-C(711)-C(712)	110.0(3)
O(62)-C(61)-O(61)	111.0(3)	N(77)-C(712)-C(77)	110.6(3)
O(62)-C(61)-C(62)	109.8(3)	N(77)-C(712)-C(711)	108.6(3)
O(61)-C(61)-C(62)	112.3(3)	C(77)-C(712)-C(711)	110.4(3)
C(63B)-C(62)-C(63A)	14(3)	C(81)-O(81)-C(813)	114.3(3)
C(63B)-C(62)-O(63)	128.2(6)	C(81)-O(82)-C(814)	113.2(3)
C(63A)-C(62)-O(63)	122.7(5)	C(82)-O(83)-C(86)	117.6(3)
C(63B)-C(62)-C(61)	122.3(6)	C(86)-O(84)-C(87)	115.8(2)
C(63A)-C(62)-C(61)	128.5(5)	N(82B)-N(81)-N(82A)	39.7(4)
O(63)-C(62)-C(61)	108.6(3)	N(82B)-N(81)-C(85)	116.0(4)
O(64)-C(67)-C(612)	105.9(3)	N(82A)-N(81)-C(85)	114.3(4)
O(64)-C(67)-C(68)	110.4(3)	N(85)-N(84)-C(810)	117.4(3)
C(612)-C(67)-C(68)	111.5(3)	N(86)-N(85)-N(84)	169.9(4)
O(65)-C(68)-C(69)	112.0(3)	N(88A)-N(87)-N(88B)	23.5(7)
O(65)-C(68)-C(67)	107.1(3)	N(88A)-N(87)-C(812)	119.0(5)
C(69)-C(68)-C(67)	111.5(3)	N(88B)-N(87)-C(812)	113.2(4)
O(66)-C(69)-C(610)	109.8(3)	O(82)-C(81)-O(81)	112.1(3)
O(66)-C(69)-C(68)	107.2(3)	O(82)-C(81)-C(82)	108.6(3)
C(610)-C(69)-C(68)	111.8(3)	O(81)-C(81)-C(82)	112.5(3)
N(64)-C(610)-C(69)	112.9(3)	C(83)-C(82)-O(83)	125.1(3)
N(64)-C(610)-C(611)	105.8(3)	C(83)-C(82)-C(81)	125.9(3)
C(69)-C(610)-C(611)	109.3(3)	O(83)-C(82)-C(81)	108.9(3)

C(82)-C(83)-C(84)	121.7(3)	C(89)-C(88)-C(87)	112.4(3)
C(83)-C(84)-C(85)	107.0(3)	O(86)-C(89)-C(810)	110.2(3)
N(81)-C(85)-C(84)	115.9(3)	O(86)-C(89)-C(88)	107.4(3)
N(81)-C(85)-C(86)	106.5(3)	C(810)-C(89)-C(88)	111.0(3)
C(84)-C(85)-C(86)	111.1(3)	N(84)-C(810)-C(89)	112.9(3)
O(84)-C(86)-O(83)	110.8(3)	N(84)-C(810)-C(811)	105.5(3)
O(84)-C(86)-C(85)	107.7(3)	C(89)-C(810)-C(811)	109.8(3)
O(83)-C(86)-C(85)	111.2(3)	C(810)-C(811)-C(812)	110.6(3)
O(84)-C(87)-C(812)	105.4(3)	N(87)-C(812)-C(87)	109.1(3)
O(84)-C(87)-C(88)	111.7(3)	N(87)-C(812)-C(811)	107.5(3)
C(812)-C(87)-C(88)	110.7(3)	C(87)-C(812)-C(811)	111.5(3)
O(85)-C(88)-C(89)	109.9(3)		
O(85)-C(88)-C(87)	107.6(3)		

Table 6. Torsion angles [°] for C14 H21 N9 O6.

C(114)-O(12)-C(11)-O(11) -70.1(4)	N(61A)-C(65A)-C(66A)-O(63) -171.2(8)
C(114)-O(12)-C(11)-C(12) 164.2(3)	C(64A)-C(65A)-C(66A)-O(63) 60.5(11)
C(113)-O(11)-C(11)-O(12) -65.3(4)	C(64A)-C(65A)-N(61A)-N(62A) -20.6(18)
C(113)-O(11)-C(11)-C(12) 57.1(4)	C(66A)-C(65A)-N(61A)-N(62A) -143.6(13)
C(16)-O(13)-C(12)-C(13) -4.5(5)	C(65A)-N(61A)-N(62A)-N(63A) -147(7)
C(16)-O(13)-C(12)-C(11) 173.7(3)	C(62)-C(63B)-C(64B)-C(65B) 7(3)
O(12)-C(11)-C(12)-C(13) 2.5(5)	C(63B)-C(64B)-C(65B)-C(66B) -41(2)
O(11)-C(11)-C(12)-C(13) -122.4(4)	C(63B)-C(64B)-C(65B)-N(61B) -162(2)
O(12)-C(11)-C(12)-O(13) -175.8(3)	C(64B)-C(65B)-C(66B)-O(64) -58.3(12)
O(11)-C(11)-C(12)-O(13) 59.4(4)	N(61B)-C(65B)-C(66B)-O(64) 65.2(10)
O(13)-C(12)-C(13)-C(14) 1.2(6)	C(64B)-C(65B)-C(66B)-O(63) 61.7(11)
C(11)-C(12)-C(13)-C(14) -176.8(3)	N(61B)-C(65B)-C(66B)-O(63) -174.9(7)
C(12)-C(13)-C(14)-C(15) 28.5(5)	C(66B)-C(65B)-N(61B)-N(62B) -90.5(14)
N(12)-N(11)-C(15)-C(14) 34.0(4)	C(64B)-C(65B)-N(61B)-N(62B) 32.4(16)
N(12)-N(11)-C(15)-C(16) -91.7(4)	C(213)-O(21)-C(21)-O(22) 66.2(4)
C(13)-C(14)-C(15)-N(11) -177.7(3)	C(213)-O(21)-C(21)-C(22) -168.1(3)
C(13)-C(14)-C(15)-C(16) -53.9(4)	C(214)-O(22)-C(21)-O(21) 62.4(4)
C(17)-O(14)-C(16)-O(13) 82.3(3)	C(214)-O(22)-C(21)-C(22) -60.8(4)
C(17)-O(14)-C(16)-C(15) -155.9(3)	C(26)-O(23)-C(22)-C(23) 21.3(4)
C(12)-O(13)-C(16)-O(14) 96.9(3)	C(26)-O(23)-C(22)-C(21) -154.5(3)
C(12)-O(13)-C(16)-C(15) -22.4(4)	O(21)-C(21)-C(22)-C(23) 0.1(5)
N(11)-C(15)-C(16)-O(14) 59.1(3)	O(22)-C(21)-C(22)-C(23) 125.3(4)
C(14)-C(15)-C(16)-O(14) -68.5(3)	O(21)-C(21)-C(22)-O(23) 175.7(3)
N(11)-C(15)-C(16)-O(13) -179.7(3)	O(22)-C(21)-C(22)-O(23) -59.1(3)
C(14)-C(15)-C(16)-O(13) 52.7(4)	O(23)-C(22)-C(23)-C(24) -2.2(5)
C(16)-O(14)-C(17)-C(112) -159.6(3)	C(21)-C(22)-C(23)-C(24) 172.8(3)
C(16)-O(14)-C(17)-C(18) 80.2(3)	C(22)-C(23)-C(24)-C(25) 13.3(5)
O(14)-C(17)-C(18)-O(15) -68.1(3)	N(22B)-N(21)-C(25)-C(24) -14.5(7)
C(112)-C(17)-C(18)-O(15) 175.2(3)	N(22A)-N(21)-C(25)-C(24) 21.3(6)
O(14)-C(17)-C(18)-C(19) 170.8(3)	N(22B)-N(21)-C(25)-C(26) -138.0(6)
C(112)-C(17)-C(18)-C(19) 54.1(4)	N(22A)-N(21)-C(25)-C(26) -102.2(6)
O(15)-C(18)-C(19)-O(16) 62.4(3)	C(23)-C(24)-C(25)-N(21) -162.8(3)
C(17)-C(18)-C(19)-O(16) -176.6(3)	C(23)-C(24)-C(25)-C(26) -40.8(4)
O(15)-C(18)-C(19)-C(110) -176.5(3)	C(27)-O(24)-C(26)-O(23) 70.0(3)
C(17)-C(18)-C(19)-C(110) -55.6(4)	C(27)-O(24)-C(26)-C(25) -170.2(3)
N(15)-N(14)-C(110)-C(19) 71.0(4)	C(22)-O(23)-C(26)-O(24) 67.6(3)
N(15)-N(14)-C(110)-C(111) -168.6(3)	C(22)-O(23)-C(26)-C(25) -49.8(4)
O(16)-C(19)-C(110)-N(14) -64.4(3)	N(21)-C(25)-C(26)-O(24) 67.4(4)
C(18)-C(19)-C(110)-N(14) 176.5(3)	C(24)-C(25)-C(26)-O(24) -59.5(4)
O(16)-C(19)-C(110)-C(111) 176.8(3)	N(21)-C(25)-C(26)-O(23) -172.5(3)
C(18)-C(19)-C(110)-C(111) 57.7(4)	C(24)-C(25)-C(26)-O(23) 60.6(4)
N(14)-C(110)-C(111)-C(112) 179.6(3)	C(26)-O(24)-C(27)-C(28) 90.5(3)
C(19)-C(110)-C(111)-C(112) -59.0(4)	C(26)-O(24)-C(27)-C(212) -148.9(3)
N(18)-N(17)-C(112)-C(17) -90.2(4)	O(24)-C(27)-C(28)-O(25) -69.4(3)
N(18)-N(17)-C(112)-C(111) 148.7(3)	C(212)-C(27)-C(28)-O(25) 173.6(3)
O(14)-C(17)-C(112)-N(17) 65.2(3)	O(24)-C(27)-C(28)-C(29) 168.8(3)
C(18)-C(17)-C(112)-N(17) -174.1(3)	C(212)-C(27)-C(28)-C(29) 51.7(4)
O(14)-C(17)-C(112)-C(111) -176.2(3)	O(25)-C(28)-C(29)-O(26) 67.5(3)
C(18)-C(17)-C(112)-C(111) -55.4(4)	C(27)-C(28)-C(29)-O(26) -173.0(3)
C(110)-C(111)-C(112)-N(17) 178.6(3)	O(25)-C(28)-C(29)-C(210) -172.9(3)
C(110)-C(111)-C(112)-C(17) 58.1(4)	C(27)-C(28)-C(29)-C(210) -53.4(4)
C(62)-C(63A)-C(64A)-C(65A) 22(4)	N(25)-N(24)-C(210)-C(29) 69.9(4)
C(63A)-C(64A)-C(65A)-N(61A) -166(2)	N(25)-N(24)-C(210)-C(211) -170.8(3)
C(63A)-C(64A)-C(65A)-C(66A) -45(2)	O(26)-C(29)-C(210)-N(24) -67.6(3)
N(61A)-C(65A)-C(66A)-O(64) 67.4(12)	C(28)-C(29)-C(210)-N(24) 174.5(3)
C(64A)-C(65A)-C(66A)-O(64) -61.0(13)	O(26)-C(29)-C(210)-C(211) 175.6(3)

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C(28)-C(29)-C(210)-C(211) 57.7(4)
N(24)-C(210)-C(211)-C(212) 177.2(3)
C(29)-C(210)-C(211)-C(212) -61.5(4)
N(28)-N(27)-C(212)-C(211) 140.1(3)
N(28)-N(27)-C(212)-C(27) -99.4(3)
C(210)-C(211)-C(212)-N(27) -179.9(3)
C(210)-C(211)-C(212)-C(27) 59.8(4)
O(24)-C(27)-C(212)-N(27)  66.2(3)
C(28)-C(27)-C(212)-N(27) -174.1(3)
O(24)-C(27)-C(212)-C(211 -174.3(3)
C(28)-C(27)-C(212)-C(211) -54.5(4)
C(314)-O(31)-C(31)-O(32) -77.0(4)
C(314)-O(31)-C(31)-C(32) 157.3(3)
C(313)-O(32)-C(31)-O(31) -63.2(4)
C(313)-O(32)-C(31)-C(32)  60.2(4)
C(36)-O(33)-C(32)-C(33)    0.7(5)
C(36)-O(33)-C(32)-C(31)  176.6(3)
O(31)-C(31)-C(32)-C(33)    2.7(5)
O(32)-C(31)-C(32)-C(33) -122.6(4)
O(31)-C(31)-C(32)-O(33) -173.1(3)
O(32)-C(31)-C(32)-O(33)   61.5(4)
O(33)-C(32)-C(33)-C(34)    1.4(6)
C(31)-C(32)-C(33)-C(34) -173.8(3)
C(32)-C(33)-C(34)-C(35)   24.7(5)
N(32B)-N(31)-C(35)-C(34)  32.1(6)
N(32A)-N(31)-C(35)-C(34)  -4.1(6)
N(32B)-N(31)-C(35)-C(36) -93.0(5)
N(32A)-N(31)-C(35)-C(36) -129.2(5)
C(33)-C(34)-C(35)-N(31) -175.4(3)
C(33)-C(34)-C(35)-C(36)  -51.5(4)
C(37)-O(34)-C(36)-O(33)   78.8(3)
C(37)-O(34)-C(36)-C(35) -158.5(3)
C(32)-O(33)-C(36)-O(34)   90.3(3)
C(32)-O(33)-C(36)-C(35)  -29.6(4)
N(31)-C(35)-C(36)-O(34)   62.3(3)
C(34)-C(35)-C(36)-O(34)  -65.6(4)
N(31)-C(35)-C(36)-O(33) -176.0(3)
C(34)-C(35)-C(36)-O(33)   56.1(4)
C(36)-O(34)-C(37)-C(312) -160.4(3)
C(36)-O(34)-C(37)-C(38)   79.2(3)
O(34)-C(37)-C(38)-O(35)  -69.0(3)
C(312)-C(37)-C(38)-O(35) 173.8(3)
O(34)-C(37)-C(38)-C(39)  168.8(3)
C(312)-C(37)-C(38)-C(39)  51.6(4)
O(35)-C(38)-C(39)-O(36)   63.8(3)
C(37)-C(38)-C(39)-O(36) -175.3(3)
O(35)-C(38)-C(39)-C(310) -174.6(3)
C(37)-C(38)-C(39)-C(310) -53.7(4)
N(35)-N(34)-C(310)-C(39)  67.2(4)
N(35)-N(34)-C(310)-C(311) -172.0(3)
O(36)-C(39)-C(310)-N(34) -64.8(4)
C(38)-C(39)-C(310)-N(34) 175.0(3)
O(36)-C(39)-C(310)-C(311) 176.8(3)
C(38)-C(39)-C(310)-C(311) 56.6(4)
N(34)-C(310)-C(311)-C(312) 178.7(3)
C(39)-C(310)-C(311)-C(312) -58.6(4)
N(38)-N(37)-C(312)-C(311) 152.2(3)
N(38)-N(37)-C(312)-C(37) -85.9(4)
C(310)-C(311)-C(312)-N(37) 179.4(3)
C(310)-C(311)-C(312)-C(37) 58.2(4)
O(34)-C(37)-C(312)-N(37)  65.0(3)
C(38)-C(37)-C(312)-N(37) -173.8(3)
O(34)-C(37)-C(312)-C(311) -175.7(3)
C(38)-C(37)-C(312)-C(311) -54.5(4)
C(414)-O(42)-C(41)-O(41)  68.0(4)
C(414)-O(42)-C(41)-C(42) -167.7(3)
C(413)-O(41)-C(41)-O(42)  60.3(4)
C(413)-O(41)-C(41)-C(42) -62.1(4)
C(46)-O(43)-C(42)-C(43)   21.5(5)
C(46)-O(43)-C(42)-C(41) -155.2(3)
O(42)-C(41)-C(42)-C(43)   -2.7(5)
O(41)-C(41)-C(42)-C(43)  121.4(4)
O(42)-C(41)-C(42)-O(43)  173.9(3)
O(41)-C(41)-C(42)-O(43)  -62.0(4)
O(43)-C(42)-C(43)-C(44)   -2.1(6)
C(41)-C(42)-C(43)-C(44)  174.1(4)
C(42)-C(43)-C(44)-C(45)   12.6(5)
N(42)-N(41)-C(45)-C(46) -147.2(4)
N(42)-N(41)-C(45)-C(44)  -24.8(5)
C(43)-C(44)-C(45)-N(41) -161.6(3)
C(43)-C(44)-C(45)-C(46)  -40.3(4)
C(47)-O(44)-C(46)-O(43)   70.4(3)
C(47)-O(44)-C(46)-C(45) -168.2(3)
C(42)-O(43)-C(46)-O(44)   67.9(4)
C(42)-O(43)-C(46)-C(45)  -51.0(4)
N(41)-C(45)-C(46)-O(44)   64.8(4)
C(44)-C(45)-C(46)-O(44)  -60.3(4)
N(41)-C(45)-C(46)-O(43) -173.9(3)
C(44)-C(45)-C(46)-O(43)   61.0(4)
C(46)-O(44)-C(47)-C(48)   90.5(3)
C(46)-O(44)-C(47)-C(412) -149.8(3)
O(44)-C(47)-C(48)-O(45)  -68.4(3)
C(412)-C(47)-C(48)-O(45) 175.3(3)
O(44)-C(47)-C(48)-C(49)  169.5(3)
C(412)-C(47)-C(48)-C(49)  53.3(4)
O(45)-C(48)-C(49)-O(46)   64.9(3)
C(47)-C(48)-C(49)-O(46) -175.2(3)
O(45)-C(48)-C(49)-C(410) -173.8(3)
C(47)-C(48)-C(49)-C(410) -54.0(4)
N(45)-N(44)-C(410)-C(411) -163.4(3)
N(45)-N(44)-C(410)-C(49)  76.5(4)
O(46)-C(49)-C(410)-N(44) -66.3(4)
C(48)-C(49)-C(410)-N(44) 174.4(3)
O(46)-C(49)-C(410)-C(411) 175.6(3)
C(48)-C(49)-C(410)-C(411) 56.2(4)
N(44)-C(410)-C(411)-C(412) 178.0(3)
C(49)-C(410)-C(411)-C(412) -59.5(4)
N(48)-N(47)-C(412)-C(411) 141.2(3)
N(48)-N(47)-C(412)-C(47) -97.9(4)
C(410)-C(411)-C(412)-N(47) -179.5(3)
C(410)-C(411)-C(412)-C(47) 59.7(4)
O(44)-C(47)-C(412)-N(47)  64.6(3)
C(48)-C(47)-C(412)-N(47) -175.7(3)
O(44)-C(47)-C(412)-C(411) -175.5(3)
C(48)-C(47)-C(412)-C(411) -55.8(4)
C(514)-O(52)-C(51)-O(51) -71.8(4)
C(514)-O(52)-C(51)-C(52) 161.3(4)
C(513)-O(51)-C(51)-O(52) -64.1(5)
C(513)-O(51)-C(51)-C(52)  58.8(5)
C(56)-O(53)-C(52)-C(53)   -0.2(11)
C(56)-O(53)-C(52)-C(51)  177.7(5)
O(52)-C(51)-C(52)-C(53)   10.6(6)
O(51)-C(51)-C(52)-C(53) -114.5(5)
O(52)-C(51)-C(52)-O(53) -167.3(5)
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O(51)-C(51)-C(52)-O(53)   67.6(6)
O(53)-C(52)-C(53)-C(54)   -0.1(10)
C(51)-C(52)-C(53)-C(54) -177.7(5)
C(52)-C(53)-C(54)-C(55)   27.7(8)
C(914)-O(92)-C(91)-O(91)  69.8(13)
C(914)-O(92)-C(91)-C(92) -161.2(10)
C(913)-O(91)-C(91)-O(92) -152.2(15)
C(913)-O(91)-C(91)-C(92)  83.4(18)
C(56)-O(93)-C(92)-C(93)    9(3)
C(56)-O(93)-C(92)-C(91) -179.1(15)
O(92)-C(91)-C(92)-C(93)  110(2)
O(91)-C(91)-C(92)-C(93) -125.3(18)
O(92)-C(91)-C(92)-O(93)  -61.6(16)
O(91)-C(91)-C(92)-O(93)   62.8(18)
O(93)-C(92)-C(93)-C(94)   -1(3)
C(91)-C(92)-C(93)-C(94) -171.6(15)
C(92)-C(93)-C(94)-C(55)   22(3)
N(52)-N(51)-C(55)-C(94)   33.6(9)
N(52)-N(51)-C(55)-C(54)   38.9(6)
N(52)-N(51)-C(55)-C(56)  -88.9(4)
C(93)-C(94)-C(55)-N(51) -169.7(12)
C(93)-C(94)-C(55)-C(54)   48(4)
C(93)-C(94)-C(55)-C(56)  -47.9(16)
C(53)-C(54)-C(55)-N(51)  179.1(4)
C(53)-C(54)-C(55)-C(94) -141(5)
C(53)-C(54)-C(55)-C(56)  -54.0(6)
C(57)-O(54)-C(56)-O(53)   75.4(4)
C(57)-O(54)-C(56)-O(93)   78.5(5)
C(57)-O(54)-C(56)-C(55) -162.0(3)
C(52)-O(53)-C(56)-O(54)   92.8(7)
C(52)-O(53)-C(56)-O(93)   64(6)
C(52)-O(53)-C(56)-C(55)  -27.3(8)
C(92)-O(93)-C(56)-O(54)   80(2)
C(92)-O(93)-C(56)-O(53) -128(9)
C(92)-O(93)-C(56)-C(55)  -37(2)
N(51)-C(55)-C(56)-O(54)   63.0(4)
C(94)-C(55)-C(56)-O(54)  -59.5(8)
C(54)-C(55)-C(56)-O(54)  -67.7(4)
N(51)-C(55)-C(56)-O(53) -173.4(5)
C(94)-C(55)-C(56)-O(53)   64.1(9)
C(54)-C(55)-C(56)-O(53)   55.9(6)
N(51)-C(55)-C(56)-O(93)  179.8(12)
C(94)-C(55)-C(56)-O(93)   57.3(13)
C(54)-C(55)-C(56)-O(93)   49.2(12)
C(56)-O(54)-C(57)-C(512) -157.5(3)
C(56)-O(54)-C(57)-C(58)   82.6(3)
O(54)-C(57)-C(58)-O(55)  -68.9(3)
C(512)-C(57)-C(58)-O(55) 174.6(3)
O(54)-C(57)-C(58)-C(59)  169.4(3)
C(512)-C(57)-C(58)-C(59)  52.9(4)
O(55)-C(58)-C(59)-O(56)   64.2(3)
C(57)-C(58)-C(59)-O(56) -175.6(3)
O(55)-C(58)-C(59)-C(510) -175.6(3)
C(57)-C(58)-C(59)-C(510) -55.3(4)
N(55)-N(54)-C(510)-C(59)  70.5(4)
N(55)-N(54)-C(510)-C(511) -170.1(3)
O(56)-C(59)-C(510)-N(54) -66.1(4)
C(58)-C(59)-C(510)-N(54) 175.4(3)
O(56)-C(59)-C(510)-C(511) 176.3(3)
C(58)-C(59)-C(510)-C(511) 57.8(4)
N(54)-C(510)-C(511)-C(512) 179.3(3)
C(59)-C(510)-C(511)-C(512) -58.7(4)
N(58)-N(57)-C(512)-C(57) -89.6(4)
N(58)-N(57)-C(512)-C(511) 148.0(4)
O(54)-C(57)-C(512)-N(57)  63.9(4)
C(58)-C(57)-C(512)-N(57) -175.6(3)
O(54)-C(57)-C(512)-C(511) -175.8(3)
C(58)-C(57)-C(512)-C(511) -55.2(4)
C(510)-C(511)-C(512)-N(57) -179.6(3)
C(510)-C(511)-C(512)-C(57) 58.8(4)
O(64)-C(66A)-O(63)-C(62)  65.3(7)
C(65A)-C(66A)-O(63)-C(62) -51.0(10)
O(64)-C(66A)-O(63)-C(66B) 97(5)
C(65A)-C(66A)-O(63)-C(66B) -19(4)
O(64)-C(66B)-O(63)-C(62)  75.1(6)
C(65B)-C(66B)-O(63)-C(62) -43.7(9)
O(64)-C(66B)-O(63)-C(66A) -75(4)
C(65B)-C(66B)-O(63)-C(66A) 167(5)
O(63)-C(66A)-O(64)-C(66B) -109(4)
C(65A)-C(66A)-O(64)-C(66B) 11(3)
O(63)-C(66A)-O(64)-C(67)  72.7(6)
C(65A)-C(66A)-O(64)-C(67) -168.0(5)
O(63)-C(66B)-O(64)-C(66A) 63(3)
C(65B)-C(66B)-O(64)-C(66A) -176(4)
O(63)-C(66B)-O(64)-C(67)  64.4(6)
C(65B)-C(66B)-O(64)-C(67) -174.2(5)
C(613)-O(62)-C(61)-O(61)  67.1(4)
C(613)-O(62)-C(61)-C(62) -168.1(3)
C(614)-O(61)-C(61)-O(62)  64.7(5)
C(614)-O(61)-C(61)-C(62) -58.6(4)
C(64B)-C(63B)-C(62)-C(63A) -60(5)
C(64B)-C(63B)-C(62)-O(63) 11(4)
C(64B)-C(63B)-C(62)-C(61) 178.8(19)
C(64A)-C(63A)-C(62)-C(63B) 107(9)
C(64A)-C(63A)-C(62)-O(63) -11(4)
C(64A)-C(63A)-C(62)-C(61) 174.7(18)
C(66A)-O(63)-C(62)-C(63B) 11(2)
C(66B)-O(63)-C(62)-C(63B)  8(2)
C(66A)-O(63)-C(62)-C(63A) 27(2)
C(66B)-O(63)-C(62)-C(63A) 23(2)
C(66A)-O(63)-C(62)-C(61) -158.1(4)
C(66B)-O(63)-C(62)-C(61) -161.3(4)
O(62)-C(61)-C(62)-C(63B)   8(2)
O(61)-C(61)-C(62)-C(63B) 132(2)
O(62)-C(61)-C(62)-C(63A)  -7(2)
O(61)-C(61)-C(62)-C(63A) 117(2)
O(62)-C(61)-C(62)-O(63)  178.3(3)
O(61)-C(61)-C(62)-O(63)  -57.7(4)
C(66A)-O(64)-C(67)-C(612) -145.9(4)
C(66B)-O(64)-C(67)-C(612) -146.1(4)
C(66A)-O(64)-C(67)-C(68)  93.3(4)
C(66B)-O(64)-C(67)-C(68)  93.1(4)
O(64)-C(67)-C(68)-O(65)  -67.3(4)
C(612)-C(67)-C(68)-O(65) 175.2(3)
O(64)-C(67)-C(68)-C(69)  169.9(3)
C(612)-C(67)-C(68)-C(69)  52.4(4)
O(65)-C(68)-C(69)-O(66)   65.3(4)
C(67)-C(68)-C(69)-O(66) -174.8(3)
O(65)-C(68)-C(69)-C(610) -174.3(3)
C(67)-C(68)-C(69)-C(610) -54.4(4)
N(65)-N(64)-C(610)-C(69)  81.0(4)
N(65)-N(64)-C(610)-C(611) -159.6(3)
O(66)-C(69)-C(610)-N(64) -66.4(4)
C(68)-C(69)-C(610)-N(64) 174.8(3)
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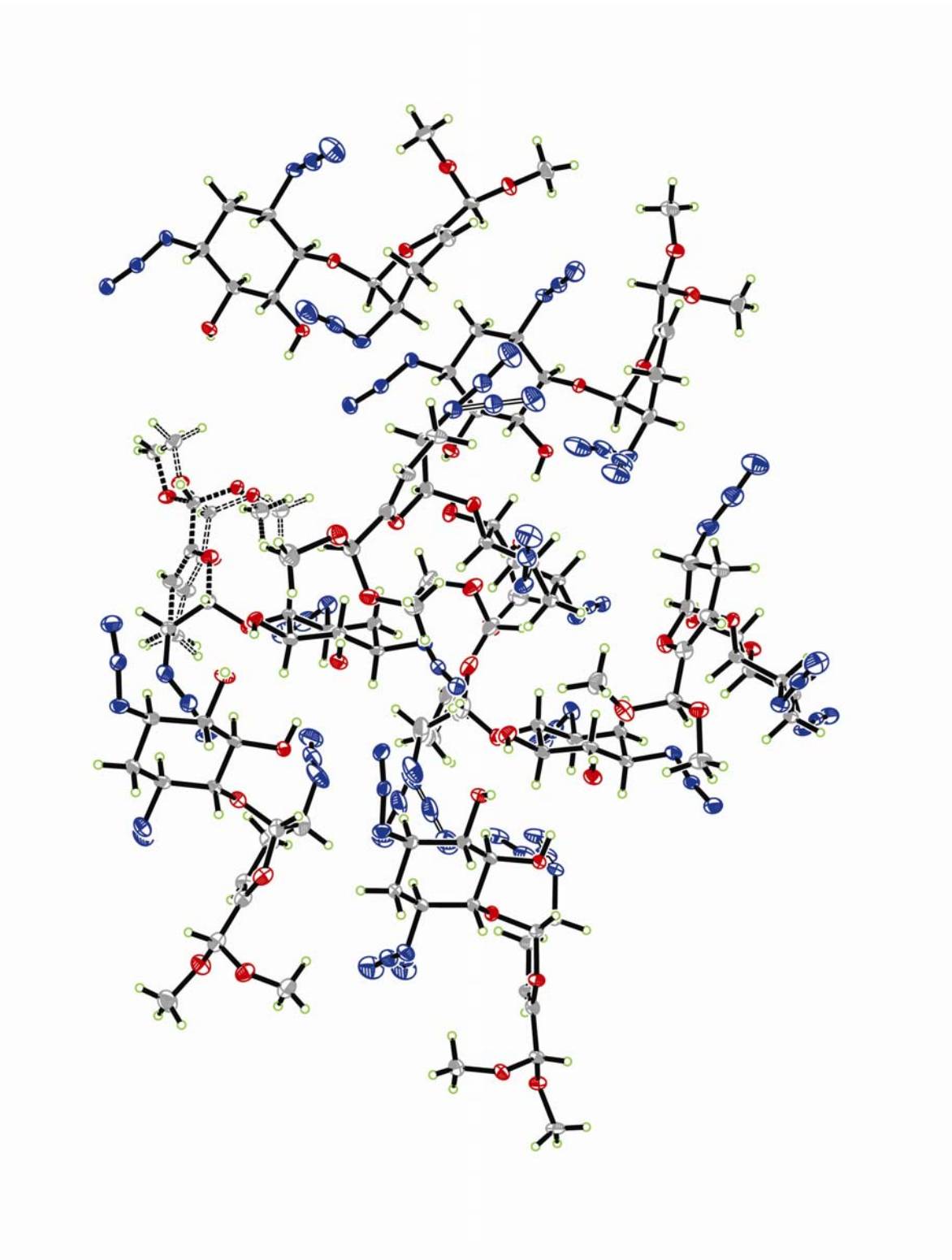
O(66)-C(69)-C(610)-C(611) 176.3(3)
C(68)-C(69)-C(610)-C(611) 57.4(4)
N(64)-C(610)-C(611)-C(612) 178.7(3)
C(69)-C(610)-C(611)-C(612) -59.5(4)
N(68)-N(67)-C(612)-C(611) 137.0(3)
N(68)-N(67)-C(612)-C(67) -101.8(4)
C(610)-C(611)-C(612)-N(67) 179.0(3)
C(610)-C(611)-C(612)-C(67) 58.5(4)
O(64)-C(67)-C(612)-N(67) 65.2(3)
C(68)-C(67)-C(612)-N(67)-174.7(3)
O(64)-C(67)-C(612)-C(611) -174.8(3)
C(68)-C(67)-C(612)-C(611) -54.7(4)
C(714)-O(72)-C(71)-O(71) 68.0(4)
C(714)-O(72)-C(71)-C(72) -168.0(3)
C(713)-O(71)-C(71)-O(72) 62.2(5)
C(713)-O(71)-C(71)-C(72) -59.7(4)
C(76)-O(73)-C(72)-C(73) 14.8(5)
C(76)-O(73)-C(72)-C(71) -162.4(3)
O(72)-C(71)-C(72)-C(73) 7.3(5)
O(71)-C(71)-C(72)-C(73) 131.1(4)
O(72)-C(71)-C(72)-O(73) -175.5(3)
O(71)-C(71)-C(72)-O(73) -51.7(4)
O(73)-C(72)-C(73)-C(74) 0.5(6)
C(71)-C(72)-C(73)-C(74) 177.3(4)
C(72)-C(73)-C(74)-C(75) 15.0(6)
N(72)-N(71)-C(75)-C(76) -135.6(4)
N(72)-N(71)-C(75)-C(74) -12.6(6)
C(73)-C(74)-C(75)-C(76) -44.2(5)
C(73)-C(74)-C(75)-N(71) -165.0(4)
C(77)-O(74)-C(76)-O(73) 75.0(3)
C(77)-O(74)-C(76)-C(75) -164.8(3)
C(72)-O(73)-C(76)-O(74) 72.8(4)
C(72)-O(73)-C(76)-C(75) -44.9(4)
N(71)-C(75)-C(76)-O(74) 65.4(4)
C(74)-C(75)-C(76)-O(74) -59.4(4)
N(71)-C(75)-C(76)-O(73) -174.3(3)
C(74)-C(75)-C(76)-O(73) 60.9(5)
C(76)-O(74)-C(77)-C(712) -148.8(3)
C(76)-O(74)-C(77)-C(78) 91.3(3)
O(74)-C(77)-C(78)-O(75) -65.2(3)
C(712)-C(77)-C(78)-O(75) 176.7(3)
O(74)-C(77)-C(78)-C(79) 172.7(3)
C(712)-C(77)-C(78)-C(79) 54.6(4)
O(75)-C(78)-C(79)-O(76) 64.3(3)
C(77)-C(78)-C(79)-O(76) -175.1(3)
O(75)-C(78)-C(79)-C(710) -174.9(3)
C(77)-C(78)-C(79)-C(710) -54.3(4)
N(75)-N(74)-C(710)-C(711) -162.6(3)
N(75)-N(74)-C(710)-C(79) 78.5(4)
O(76)-C(79)-C(710)-N(74) -68.6(4)
C(78)-C(79)-C(710)-N(74) 172.9(3)
O(76)-C(79)-C(710)-C(711) 174.7(3)
C(78)-C(79)-C(710)-C(711) 56.1(4)
N(74)-C(710)-C(711)-C(712) 179.7(3)
C(79)-C(710)-C(711)-C(712) -59.7(4)
N(78)-N(77)-C(712)-C(77) -94.0(4)
N(78)-N(77)-C(712)-C(711) 144.7(3)
O(74)-C(77)-C(712)-N(77) 61.2(3)
C(78)-C(77)-C(712)-N(77) -177.9(3)
O(74)-C(77)-C(712)-C(711) -178.6(3)
C(78)-C(77)-C(712)-C(711) -57.7(4)
C(710)-C(711)-C(712)-N(77) -177.3(3)
C(710)-C(711)-C(712)-C(77) 61.3(4)
C(814)-O(82)-C(81)-O(81) -73.1(4)
C(814)-O(82)-C(81)-C(82) 162.0(3)
C(813)-O(81)-C(81)-O(82) -61.8(4)
C(813)-O(81)-C(81)-C(82) 60.9(4)
C(86)-O(83)-C(82)-C(83) 0.2(5)
C(86)-O(83)-C(82)-C(81) 176.3(3)
O(82)-C(81)-C(82)-C(83) 2.6(5)
O(81)-C(81)-C(82)-C(83) -122.0(4)
O(82)-C(81)-C(82)-O(83) -173.3(3)
O(81)-C(81)-C(82)-O(83) 62.0(4)
O(83)-C(82)-C(83)-C(84) 1.5(6)
C(81)-C(82)-C(83)-C(84) -173.8(3)
C(82)-C(83)-C(84)-C(85) 25.5(5)
N(82B)-N(81)-C(85)-C(84) -18.9(6)
N(82A)-N(81)-C(85)-C(84) 25.1(6)
N(82B)-N(81)-C(85)-C(86) -143.1(5)
N(82A)-N(81)-C(85)-C(86) -99.0(5)
C(83)-C(84)-C(85)-N(81) -174.4(3)
C(83)-C(84)-C(85)-C(86) -52.7(4)
C(87)-O(84)-C(86)-O(83) 81.0(3)
C(87)-O(84)-C(86)-C(85) -157.2(3)
C(82)-O(83)-C(86)-O(84) 90.7(3)
C(82)-O(83)-C(86)-C(85) -29.1(4)
N(81)-C(85)-C(86)-O(84) 62.2(3)
C(84)-C(85)-C(86)-O(84) -64.8(4)
N(81)-C(85)-C(86)-O(83) -176.2(3)
C(84)-C(85)-C(86)-O(83) 56.8(4)
C(86)-O(84)-C(87)-C(812) -158.4(3)
C(86)-O(84)-C(87)-C(88) 81.4(3)
O(84)-C(87)-C(88)-O(85) -69.5(3)
C(812)-C(87)-C(88)-O(85) 173.4(3)
O(84)-C(87)-C(88)-C(89) 169.3(3)
C(812)-C(87)-C(88)-C(89) 52.3(4)
O(85)-C(88)-C(89)-O(86) 64.8(3)
C(87)-C(88)-C(89)-O(86) -175.4(3)
O(85)-C(88)-C(89)-C(810) -174.8(3)
C(87)-C(88)-C(89)-C(810) -54.9(4)
N(85)-N(84)-C(810)-C(89) 69.6(4)
N(85)-N(84)-C(810)-C(811) -170.4(3)
O(86)-C(89)-C(810)-N(84) -65.9(4)
C(88)-C(89)-C(810)-N(84) 175.3(3)
O(86)-C(89)-C(810)-C(811) 176.7(3)
C(88)-C(89)-C(810)-C(811) 57.8(4)
N(84)-C(810)-C(811)-C(812) 178.7(3)
C(89)-C(810)-C(811)-C(812) -59.4(4)
N(88A)-N(87)-C(812)-C(87) -117.3(6)
N(88B)-N(87)-C(812)-C(87) -91.9(6)
N(88A)-N(87)-C(812)-C(811) 121.6(6)
N(88B)-N(87)-C(812)-C(811) 147.0(5)
O(84)-C(87)-C(812)-N(87) 67.0(3)
C(88)-C(87)-C(812)-N(87) -172.1(3)
O(84)-C(87)-C(812)-C(811) -174.4(3)
C(88)-C(87)-C(812)-C(811) -53.5(4)
C(810)-C(811)-C(812)-N(87) 177.4(3)
C(810)-C(811)-C(812)-C(87) 57.8(4)

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C14 H21 N9 O6.

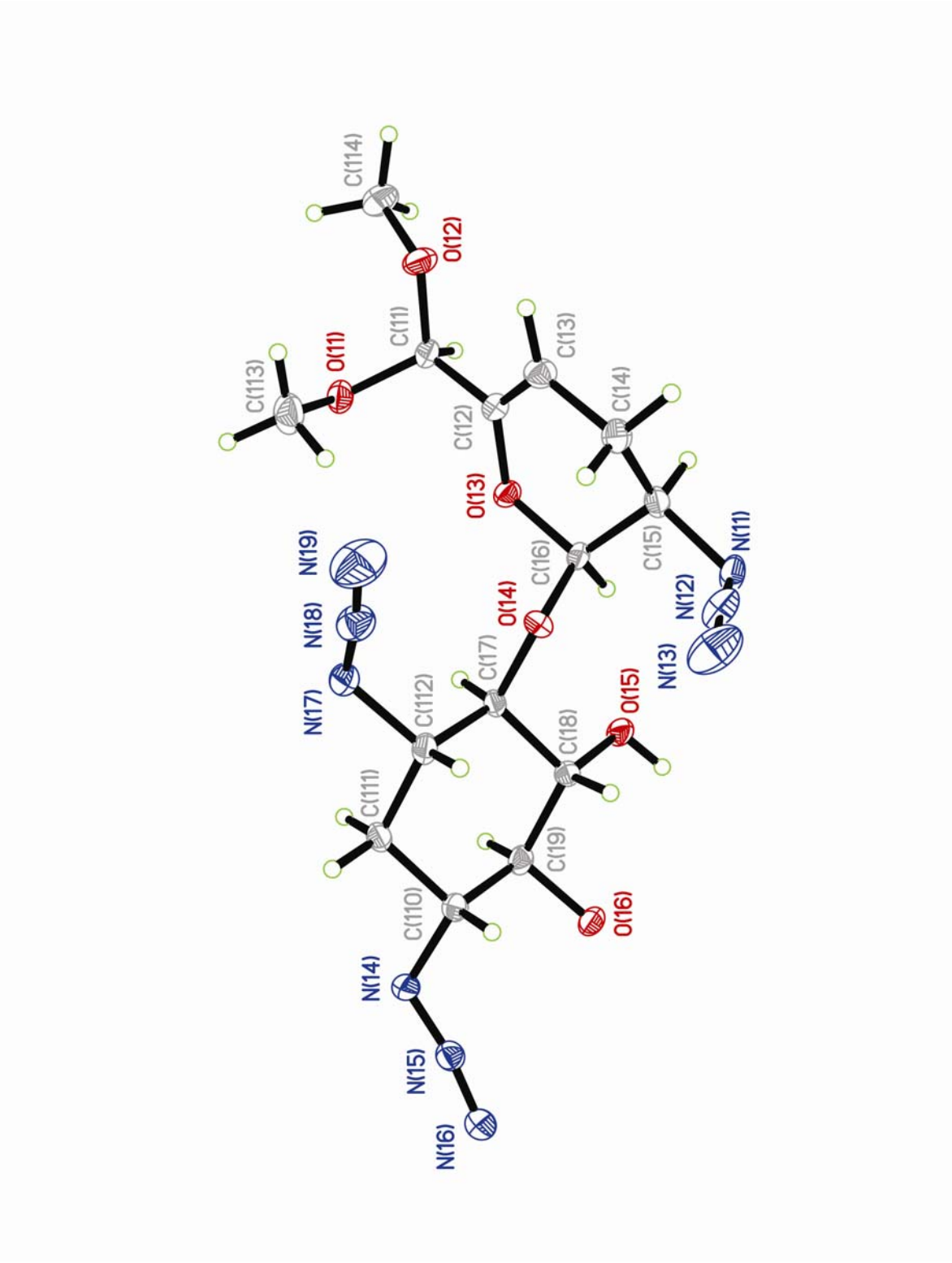
D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(15)-H(15)	O(46)#1	0.84	2.11	2.913(3)	159.6
O(16)-H(16)	O(81)#2	0.84	1.95	2.777(3)	169.2
O(25)-H(25)	O(36)	0.84	2.01	2.843(3)	170.5
O(26)-H(26)	O(71)#3	0.84	1.9	2.722(3)	167.4
O(35)-H(35)	O(26)	0.84	2.09	2.871(3)	155.4
O(36)-H(36)	O(61)	0.84	1.87	2.705(4)	170
O(45)-H(45)	O(16)#4	0.84	2.07	2.876(3)	161
O(46)-H(46)	O(51)#4	0.84	1.94	2.743(4)	160
O(46)-H(46)	O(91)#4	0.84	2.09	2.841(12)	149.5
O(55)-H(55)	O(76)	0.84	2.14	2.941(3)	158.6
O(56)-H(56)	O(32)	0.84	1.95	2.751(3)	158.2
O(65)-H(65)	O(86)	0.84	2.09	2.867(3)	152.7
O(66)-H(66)	O(41)	0.84	1.99	2.753(4)	150.8
O(75)-H(75)	O(56)	0.84	2.08	2.887(3)	159.8
O(76)-H(76)	O(11)#5	0.84	1.97	2.789(3)	163.6
O(85)-H(85)	O(66)	0.84	2.05	2.866(3)	162.8
O(86)-H(86)	O(22)#5	0.84	1.91	2.732(3)	164.7

Symmetry transformations used to generate equivalent atoms:

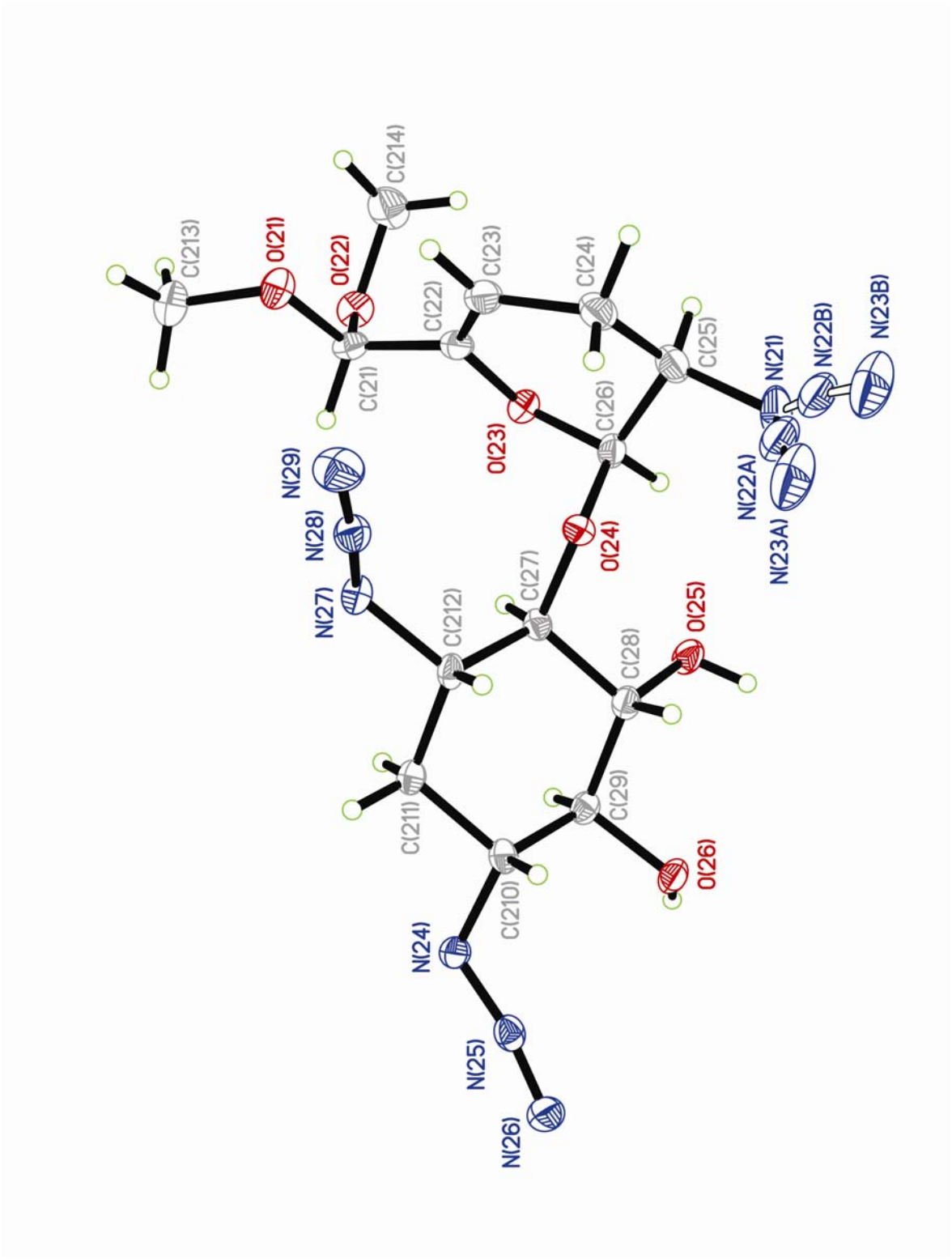
#1 x,y-1,z #2 x,y-1,z+1 #3 x,y,z+1
#4 x,y+1,z #5 x,y,z-1



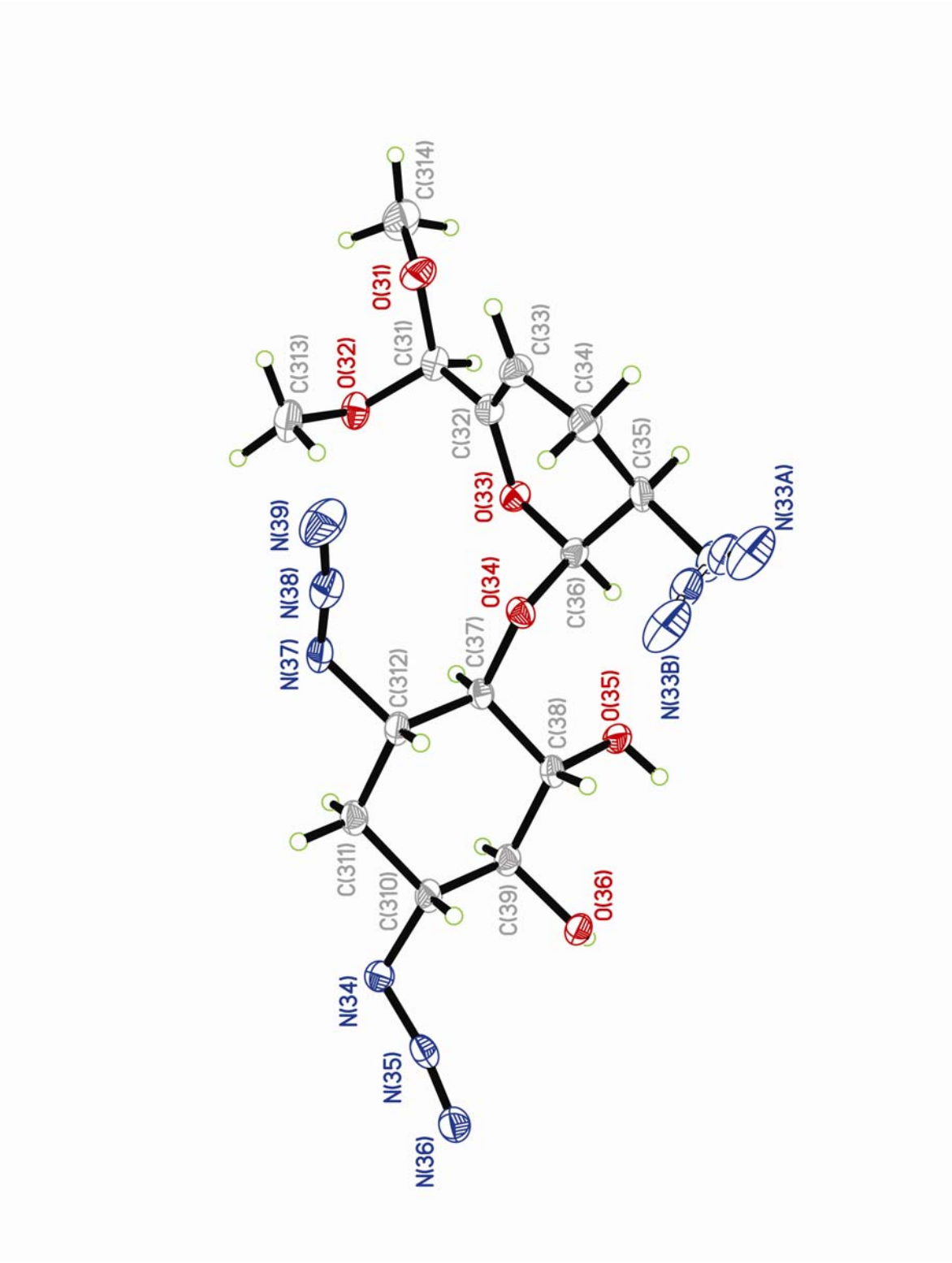
ORTEP (Asymmetric unit) view of the C14 H21 N9 O6 compound. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



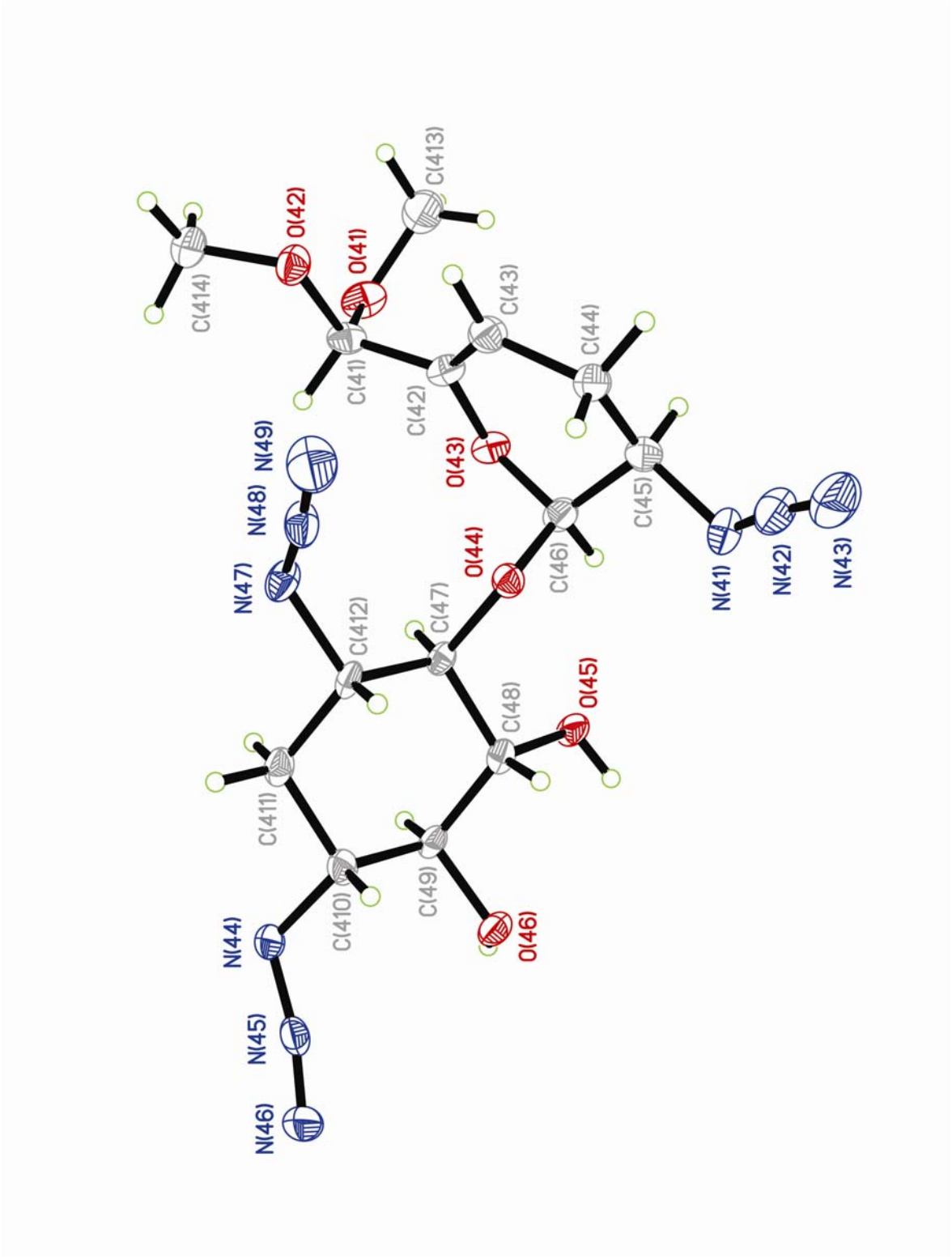
ORTEP 1 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



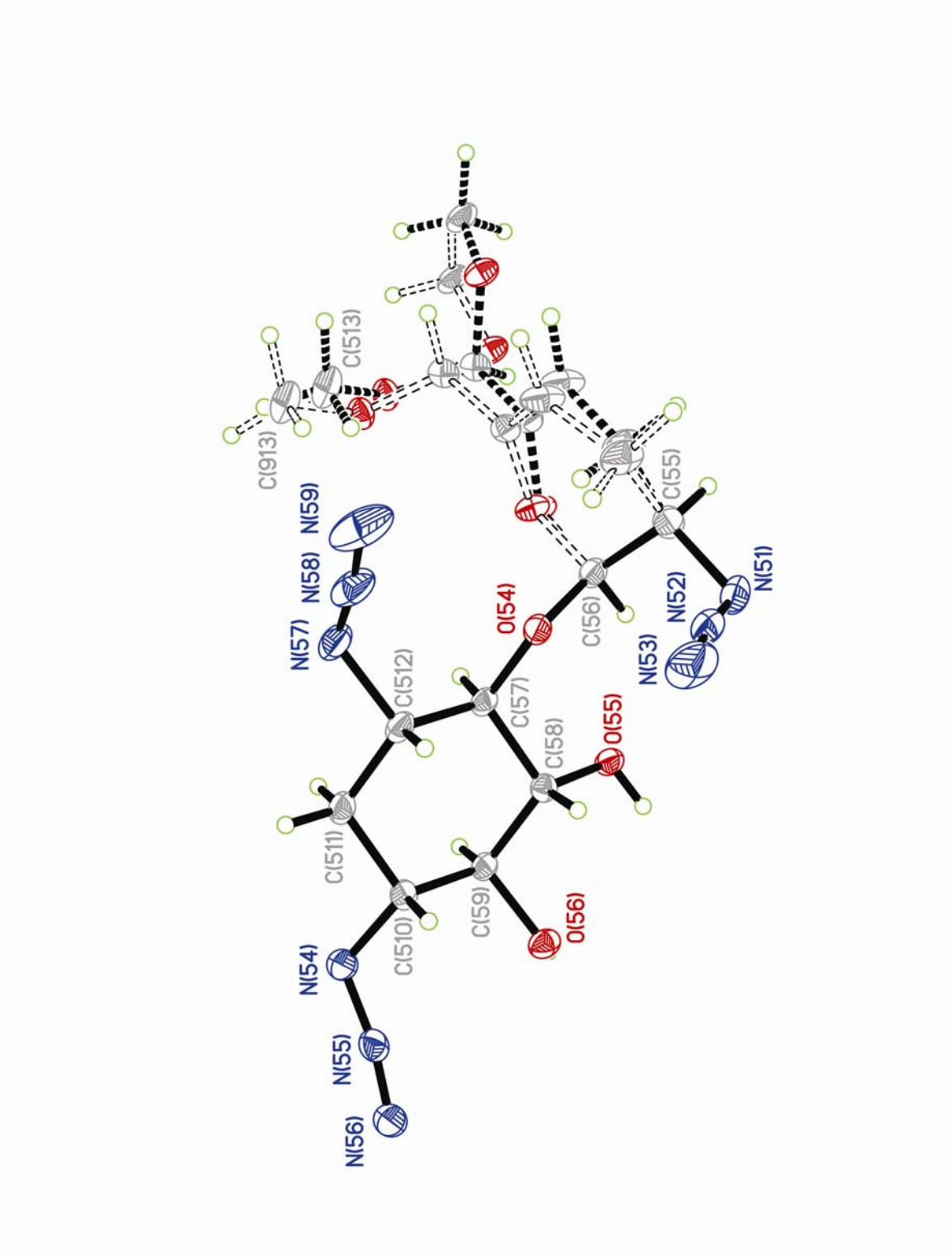
ORTEP 2 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



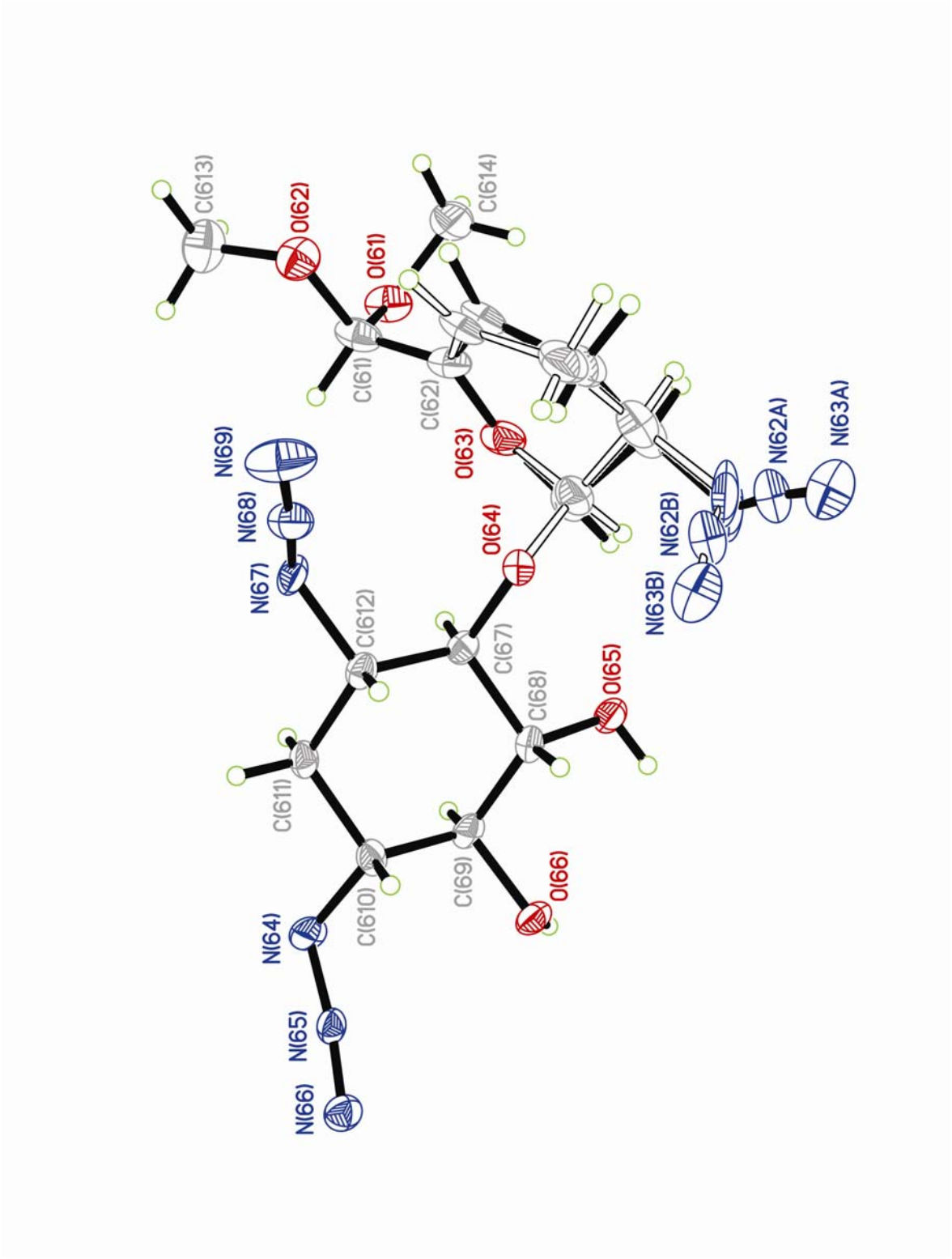
ORTEP 3 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



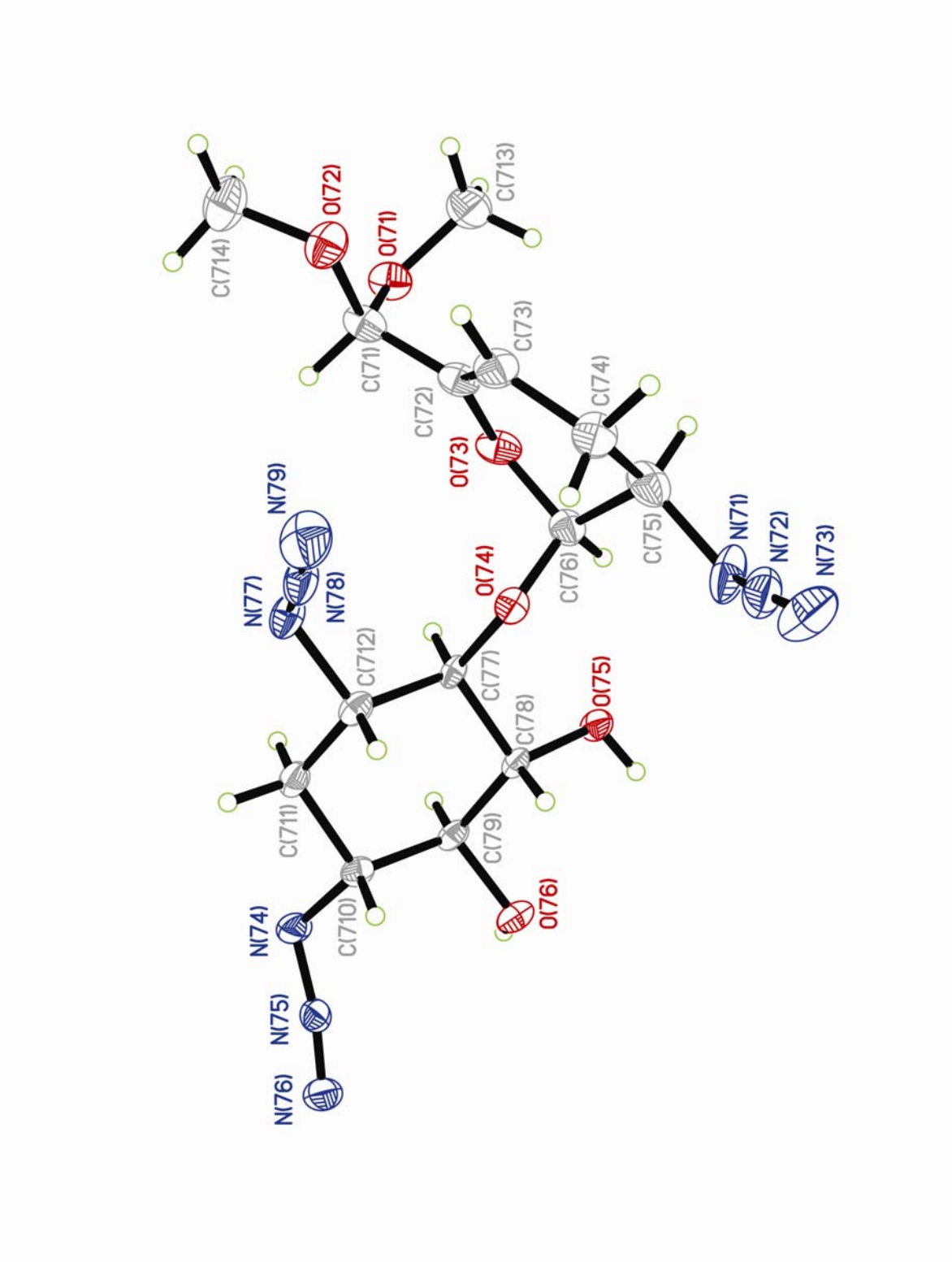
ORTEP 4 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



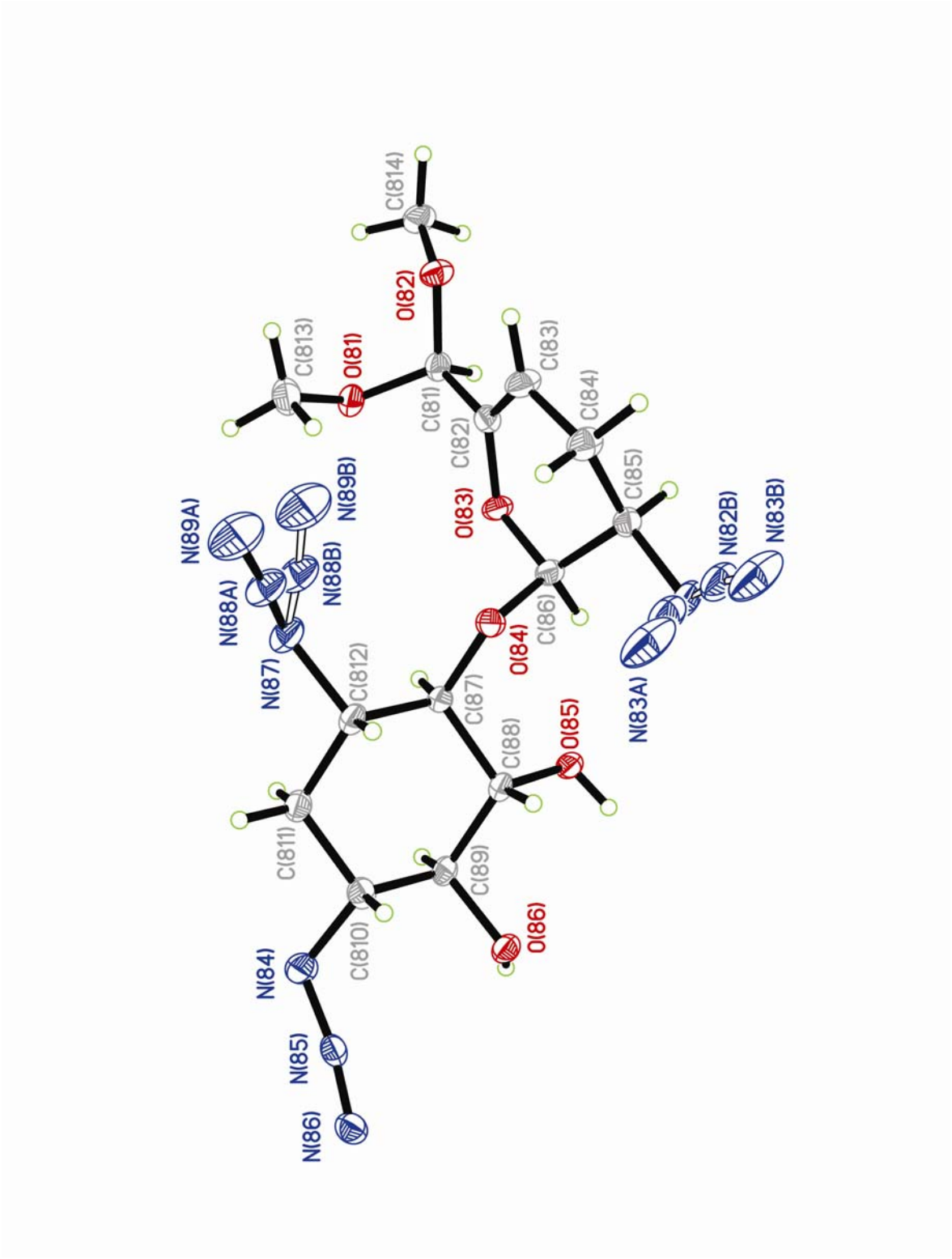
ORTEP 5 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP 6 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP 7 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP 8 view of the C14 H21 N9 O6 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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checkCIF/PLATON (standard)

Structure factors have been supplied for datablock(s) bent52

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Structure factor report

Datablock: bent52

Bond precision: C-C = 0.0060 A Wavelength=1.54178
Cell: a=15.8942(5) b=16.2322(5) c=17.6688(6)
alpha=89.748(1) beta=72.741(2) gamma=63.537(1)
Temperature: 150 K

	Calculated	Reported
Volume	3853.3(2)	3853.3(2)
Space group	P 1	P1
Hall group	P 1	P 1
Moiety formula	C14 H21 N9 O6	C14 H21 N9 O6
Sum formula	C14 H21 N9 O6	C14 H21 N9 O6
Mr	411.40	411.40
Dx,g cm-3	1.418	1.418
Z	8	8
Mu (mm-1)	0.966	0.966
F000	1728.0	1728.0
F000'	1734.12	
h,k,lmax	18,18,20	18,18,20
Nref	12820[25640]	20234
Tmin,Tmax	0.748,0.944	0.812,0.944
Tmin'	0.706	

Correction method= MULTI-SCAN
Data completeness= 1.58/0.79 Theta(max)= 64.120
R(reflections)= 0.0440(16661) wR2(reflections)= 0.1117(20234)
S = 0.985 Npar= 2194

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low 0.955

Author Response: Due to geometrical constraints of the instrument and the use of copper radiation, we obtain consistently a data completeness lower than 100% in dependence of the crystal system and the orientation of the mounted crystal, even with appropriate data collection routines. Typical values for data completeness range from 83-92% for triclinic, 85-97% for monoclinic and 85-98% for all other crystal systems. (Note: This comment is routinely included into the CIF-file and can be ignored if the data completeness is satisfactory.)

Alert level C

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5836

Author Response: Low diffraction was observed for this crystal and was especially low for high angles. Many solvent systems were tested for recrystallization. The best crystal was chosen and its size was in the limits of the diffractometer. X-ray measurements were acquired at 150K with optimized radiation exposure time and intensity. Low diffraction is also a consequence of disorder present in some molecules and the large asymmetric unit that contains 8 molecules. The final structure was satisfactory for confirming the desired chemical information with R1 = 0.0440 and wR2=0.1118.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0060 Ang

Author Response: See response for THETM01 Alert 3 C.

PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.584 571

Author Response: See response for PLAT029 Alert 3 B and THETM01 Alert 3 C.

PLAT915_ALERT_3_C Low Friedel Pair Coverage ..... 62 Perc.

Author Response: Absolute stereochemistry is known and confirmed with flack parameter.

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is
correct. If it is not, please give the correct count in the
_publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 64.12
From the CIF: _reflns_number_total 20234
Count of symmetry unique reflns 12820
Completeness (_total/calc) 157.83%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 7414
Fraction of Friedel pairs measured 0.578
Are heavy atom types Z>Si present no
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 75
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 31
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 10 Perc.
PLAT791_ALERT_4_G Note: The Model has Chirality at C15 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C16 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C17 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C18 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C19 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C25 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C26 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C27 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C28 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C29 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C35 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C36 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C37 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C38 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C39 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C45 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C46 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C47 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C48 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C49 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C57 (Verify) R
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PLAT791_ALERT_4_G Note: The Model has Chirality at C59 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C62 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C65B (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C66B (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C67 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C68 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C69 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C75 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C76 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C77 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C78 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C79 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C85 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C86 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C87 (Verify) R
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PLAT791_ALERT_4_G Note: The Model has Chirality at C610 (Verify) R
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PLAT791_ALERT_4_G Note: The Model has Chirality at C710 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C712 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C810 (Verify) R

PLAT791_ALERT_4_G Note: The Model has Chirality at C812 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C65A (Verify) R
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 447
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 55 Perc.

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
62 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
8 ALERT type 3 Indicator that the structure quality may be low
57 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

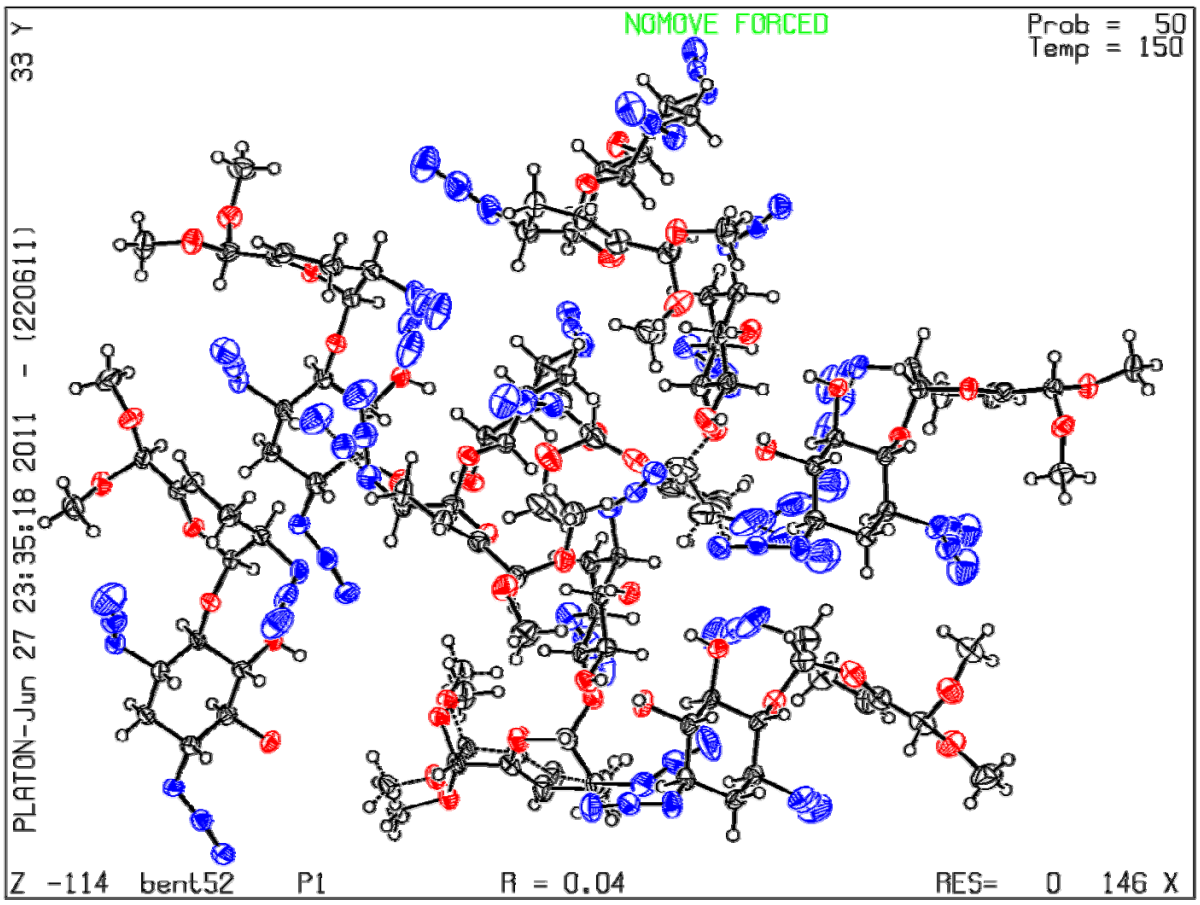
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/06/2011; check.def file version of 22/06/2011

Datablock bent52 - ellipsoid plot



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Université de Montréal

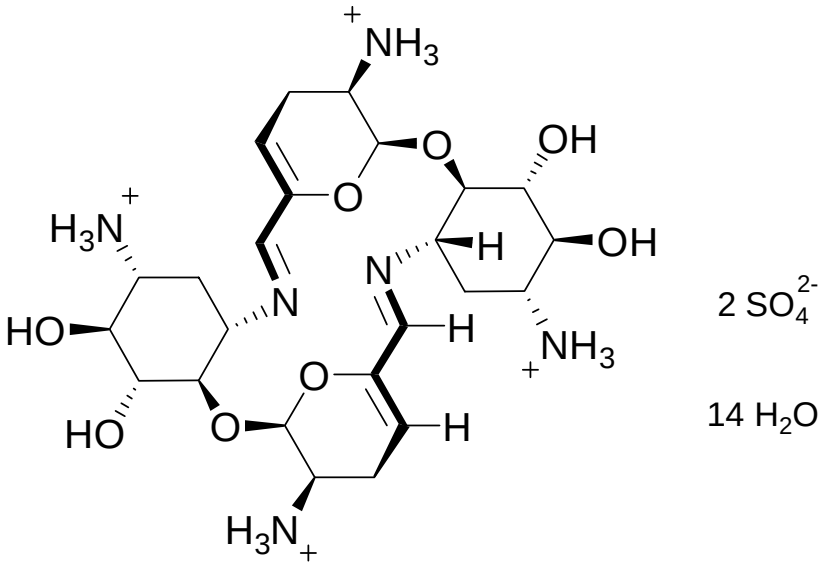
CRYSTAL AND MOLECULAR STRUCTURE OF

C24 H42 N6 O8 • 2(S O4) • 14(H2 O) COMPOUND (bent66)

Equipe Hanessian

Département de chimie, Université de Montréal,

C.P. 6128, Succ. Centre-Ville, Montréal, Québec, H3C 3J7 (Canada)



2 SO_4^{2-}

14 H_2O

Measured at 200K in monoclinic crystal system
(See phase transition to orthorhombic crystal system measured at 170K)

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C24 H70 N6 O30 S2.

Identification code	bent663
Empirical formula (ions and solvents)	C24 H42 N6 O8 • 2(S O4) • 14(H2 O)
Empirical formula	C24 H70 N6 O30 S2
Formula weight	986.98
Temperature	200K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P21
Unit cell dimensions	a = 6.8516(4) Å α = 90° b = 26.1435(15) Å β = 102.975(3)° c = 12.6653(7) Å γ = 90°
Volume	2210.7(2)Å^3
Z	2
Density (calculated)	1.483 g/cm^3
Absorption coefficient	2.018 mm^{-1}
F(000)	1056
Crystal size	0.35 x 0.09 x 0.03 mm
Theta range for data collection	3.38 to 53.69°
Index ranges	$-7 \le h \le 6$, $0 \le k \le 27$, $0 \le \ell \le 13$
Reflections collected	28784
Independent reflections	5428 [R_{int} = 0.000]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9413 and 0.6632
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5428 / 572 / 689
Goodness-of-fit on F^2	1.077
Final R indices [I>2sigma(I)]	R_1 = 0.0437, wR_2 = 0.1022
R indices (all data)	R_1 = 0.0524, wR_2 = 0.1060

Absolute structure parameter	0.07(2)
Largest diff. peak and hole	0.225 and -0.231 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C24 H70 N6 O30 S2.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
O(11)	1	3510(4)	9281(1)	2195(2)	30(1)
O(12)	1	863(4)	8720(1)	2207(2)	31(1)
O(13)	1	1519(5)	9818(1)	277(3)	43(1)
O(14)	1	4196(5)	10166(1)	-1041(3)	37(1)
N(11)	1	7249(6)	9473(2)	-1322(3)	39(1)
N(12)	1	2033(6)	10026(1)	3374(3)	36(1)
N(13)	1	6070(5)	8472(1)	1757(3)	29(1)
C(11)	1	6534(7)	9501(2)	-304(4)	32(1)
C(12)	1	6705(7)	8972(2)	245(4)	32(1)
C(13)	1	6022(7)	8995(2)	1305(4)	30(1)
C(14)	1	3881(7)	9204(2)	1129(4)	30(1)
C(15)	1	3607(7)	9702(2)	491(4)	30(1)
C(16)	1	4366(7)	9673(2)	-537(4)	32(1)
C(11')	1	1517(7)	9247(2)	2272(4)	31(1)
C(12')	1	1414(7)	9474(2)	3366(4)	31(1)
C(13')	1	2659(8)	9182(2)	4295(4)	36(1)
C(14')	1	2224(7)	8626(2)	4119(4)	37(1)
C(15')	1	1426(7)	8431(2)	3155(4)	32(1)
C(16')	1	1045(7)	7883(2)	2981(4)	32(1)
O(21)	1	3750(4)	7009(1)	3151(2)	30(1)
O(22)	1	6208(4)	7518(1)	2681(2)	30(1)
O(23)	1	4153(5)	6062(1)	2108(3)	41(1)
O(24)	1	430(5)	5528(1)	1223(2)	35(1)
N(21)	1	-2942(6)	6150(2)	238(3)	37(1)
N(22)	1	6368(5)	6488(1)	4733(3)	33(1)
N(23)	1	611(5)	7666(1)	2065(3)	30(1)
C(21)	1	-1361(7)	6338(2)	1176(4)	35(1)
C(22)	1	-1119(7)	6917(2)	1108(4)	35(1)
C(23)	1	392(6)	7105(2)	2100(4)	29(1)
C(24)	1	2412(7)	6849(2)	2141(4)	30(1)
C(25)	1	2255(7)	6264(2)	2137(4)	32(1)
C(26)	1	629(7)	6076(2)	1178(4)	33(1)
C(21')	1	5772(7)	7043(2)	3136(4)	30(1)
C(22')	1	6912(7)	6995(2)	4315(4)	31(1)
C(23')	1	6434(7)	7429(2)	5006(4)	38(1)
C(24')	1	6574(6)	7923(2)	4416(4)	31(1)
C(25')	1	6448(6)	7944(2)	3365(4)	31(1)
C(26')	1	6456(7)	8430(2)	2782(4)	34(1)
O(31)	1	1364(7)	7455(2)	6246(4)	82(1)
O(32)	1	748(5)	8010(2)	-55(3)	54(1)
O(33)	1	1506(6)	8497(2)	6663(3)	61(1)
O(34)	1	4734(6)	7772(1)	15(3)	56(1)
O(35)	1	5648(6)	8685(2)	7153(4)	62(1)
O(36)	1	3848(6)	5285(2)	6571(3)	62(1)
O(37)	1	588(6)	8845(2)	8616(3)	57(1)
O(38)	1	2450(6)	6528(2)	5148(3)	58(1)
O(39)	1	1465(6)	5276(2)	8239(3)	64(1)
O(40)	1	3720(6)	6776(2)	9764(3)	55(1)

O(41)	1	7131(6)	7806(2)	8468(3)	59(1)
O(42)	1	8159(7)	9075(2)	5659(4)	63(1)
O(43)	1	3834(5)	5104(2)	3211(3)	48(1)
O(44)	1	3741(6)	6266(2)	7270(4)	70(1)
S(1)	1	9182(2)	5399(1)	3947(1)	37(1)
O(51)	1	9407(5)	5967(1)	3871(3)	48(1)
O(52)	1	8752(5)	5186(1)	2857(3)	47(1)
O(53)	1	11058(5)	5177(1)	4579(3)	52(1)
O(54)	1	7520(5)	5303(1)	4471(3)	46(1)
S(2)	1	8865(2)	6467(1)	7714(1)	45(1)
O(61)	0.920(4)	8636(8)	6209(2)	6677(3)	55(1)
O(62)	0.920(4)	9075(6)	6092(2)	8573(3)	61(1)
O(63)	0.920(4)	7126(5)	6798(2)	7718(4)	61(1)
O(64)	0.920(4)	10688(5)	6789(2)	7900(3)	56(1)
O(71)	0.080(4)	8550(70)	6194(15)	6695(19)	54(6)
O(72)	0.080(4)	7290(40)	6356(14)	8270(30)	56(6)
O(73)	0.080(4)	8970(50)	7024(5)	7540(30)	65(5)
O(74)	0.080(4)	10830(30)	6312(14)	8410(30)	55(6)

Table 3. Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2\ x\ 10^3$) for C24 H70 N6 O30 S2.

	Occ.	x	y	z	U_{eq}
H(13D)	1	1315	10103	-34	64
H(14C)	1	3458	10145	-1666	56
H(11A)	1	8566	9383	-1169	59
H(11B)	1	7099	9784	-1653	59
H(11C)	1	6523	9235	-1769	59
H(12A)	1	3343	10045	3340	54
H(12B)	1	1865	10177	3994	54
H(12C)	1	1264	10189	2792	54
H(11D)	1	7375	9751	197	39
H(12D)	1	5871	8722	-246	38
H(12E)	1	8113	8854	387	38
H(13A)	1	6951	9220	1827	36
H(14A)	1	2922	8943	734	36
H(15A)	1	4356	9978	959	36
H(16A)	1	3529	9423	-1042	38
H(11E)	1	651	9449	1676	37
H(12F)	1	-12	9462	3434	38
H(13B)	1	4099	9247	4339	43
H(13C)	1	2338	9293	4983	43
H(14B)	1	2531	8402	4725	45
H(16B)	1	1129	7675	3604	38
H(23D)	1	4194	5751	2275	62
H(24C)	1	290	5442	1841	53
H(21A)	1	-2440	6143	-369	55
H(21B)	1	-4017	6363	131	55
H(21C)	1	-3327	5829	383	55
H(22A)	1	5042	6487	4739	50
H(22B)	1	7106	6438	5418	50
H(22C)	1	6626	6233	4295	50
H(21D)	1	-1770	6253	1865	41
H(22D)	1	-656	7005	445	42
H(22E)	1	-2426	7087	1069	42
H(23C)	1	-83	7010	2765	35
H(24B)	1	2958	6965	1512	36
H(25A)	1	1898	6151	2825	38
H(26)	1	1038	6167	491	39
H(21E)	1	6143	6754	2704	36
H(22F)	1	8381	6997	4342	37
H(23A)	1	5069	7387	5132	45
H(23B)	1	7398	7432	5717	45
H(24A)	1	6762	8232	4819	37
H(26A)	1	6771	8732	3200	41
H(31A)	1	1800(90)	7201(15)	5910(40)	105
H(31B)	1	1260(100)	7330(20)	6870(30)	105
H(32A)	1	360(50)	7910(30)	520(30)	105
H(32B)	1	2030(20)	7937(19)	70(40)	105
H(33A)	1	1140(80)	8176(6)	6630(60)	105
H(33B)	1	510(50)	8662(15)	6247(19)	105
H(34A)	1	5460(60)	7838(11)	-450(30)	105
H(34B)	1	5330(70)	7930(20)	610(20)	105
H(35A)	1	4347(14)	8670(20)	7060(60)	105
H(35B)	1	6100(70)	8392(13)	7440(60)	105

H(36A)	1	3140(80)	5240(20)	5910(20)	105
H(36B)	1	3990(70)	5616(5)	6660(30)	105
H(37A)	1	830(90)	8750(20)	8000(20)	105
H(37B)	1	730(100)	8571(12)	9020(30)	105
H(38A)	1	1580(70)	6321(17)	4760(40)	105
H(38B)	1	2880(80)	6369(18)	5760(20)	105
H(39A)	1	2110(70)	5370(20)	7750(30)	105
H(39B)	1	1020(90)	5557(12)	8470(50)	105
H(40A)	1	2590(50)	6750(20)	9290(40)	105
H(40B)	1	4210(80)	7073(12)	9650(50)	105
H(41A)	1	8320(20)	7700(20)	8430(50)	105
H(41B)	1	6290(30)	7603(9)	8043(16)	105
H(42A)	1	7340(70)	9050(20)	6100(40)	105
H(42B)	1	8150(100)	9397(7)	5480(50)	105
H(43A)	1	5060(20)	5140(30)	3590(30)	105
H(43B)	1	3060(50)	5160(30)	3660(30)	105
H(44A)	1	4720(40)	6340(30)	7820(30)	105
H(44B)	1	2650(40)	6360(30)	7460(30)	105

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C24 H70 N6 O30 S2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
O(11)	29(1)	27(1)	34(1)	-1(1)	7(1)	-2(1)
O(12)	32(1)	26(1)	35(1)	-2(1)	5(1)	-1(1)
O(13)	41(2)	41(2)	51(2)	17(2)	19(2)	14(2)
O(14)	43(2)	24(2)	42(2)	11(2)	6(2)	3(2)
N(11)	37(2)	37(3)	46(3)	7(2)	16(2)	9(2)
N(12)	45(2)	26(2)	38(2)	-4(2)	9(2)	-2(2)
N(13)	31(2)	21(2)	36(3)	6(2)	9(2)	6(2)
C(11)	40(3)	29(3)	30(3)	6(2)	13(2)	0(2)
C(12)	34(3)	24(3)	37(3)	6(2)	7(2)	0(2)
C(13)	28(1)	27(1)	34(1)	0(1)	7(1)	-2(1)
C(14)	28(1)	27(1)	34(1)	0(1)	7(1)	-1(1)
C(15)	29(1)	27(1)	35(1)	0(1)	7(1)	0(1)
C(16)	32(3)	29(3)	36(3)	2(2)	9(2)	-2(2)
C(11')	30(1)	26(1)	35(1)	-2(1)	6(1)	-1(1)
C(12')	31(1)	27(1)	36(1)	-2(1)	6(1)	-2(1)
C(13')	53(3)	26(3)	30(3)	-3(2)	14(3)	-6(2)
C(14')	37(3)	43(3)	34(3)	1(3)	13(2)	-1(3)
C(15')	30(3)	37(3)	29(3)	3(2)	10(2)	3(2)
C(16')	27(3)	31(3)	36(3)	3(2)	5(2)	0(2)
O(21)	28(1)	27(1)	34(1)	1(1)	5(1)	0(1)
O(22)	31(1)	27(1)	33(1)	3(1)	5(1)	-2(1)
O(23)	33(2)	28(2)	61(2)	0(2)	5(2)	2(2)
O(24)	44(2)	23(2)	39(2)	-3(1)	10(2)	-3(1)
N(21)	38(2)	33(3)	38(2)	1(2)	3(2)	-6(2)
N(22)	38(2)	27(2)	32(2)	2(2)	3(2)	2(2)
N(23)	28(2)	25(2)	36(3)	-1(2)	6(2)	4(2)
C(21)	40(3)	32(3)	30(3)	1(2)	3(2)	-3(2)
C(22)	32(3)	35(3)	39(3)	-5(2)	11(2)	-3(2)
C(23)	26(3)	30(3)	33(3)	2(2)	8(2)	-2(2)
C(24)	30(3)	32(3)	26(3)	-2(2)	4(2)	-4(2)
C(25)	31(3)	28(3)	38(3)	4(2)	11(2)	0(2)
C(26)	36(3)	25(3)	37(3)	0(2)	8(2)	-5(2)
C(21')	29(1)	26(1)	34(1)	3(1)	5(1)	-1(1)
C(22')	30(1)	26(1)	35(1)	3(1)	5(1)	-2(1)
C(23')	43(3)	37(3)	33(3)	3(2)	7(2)	-1(3)
C(24')	27(3)	33(3)	30(3)	-2(2)	0(2)	-5(2)
C(25')	25(3)	25(3)	39(3)	-2(2)	0(2)	0(2)
C(26')	31(3)	34(3)	39(3)	-1(2)	10(2)	2(2)
O(31)	91(3)	61(3)	94(4)	5(3)	23(3)	6(3)
O(32)	57(2)	51(2)	51(2)	5(2)	8(2)	-1(2)
O(33)	59(3)	60(3)	62(3)	3(2)	11(2)	3(2)
O(34)	73(3)	34(2)	57(2)	-4(2)	9(2)	-3(2)
O(35)	51(2)	63(3)	69(3)	1(2)	8(2)	1(2)
O(36)	59(3)	66(3)	58(3)	3(2)	5(2)	5(2)
O(37)	51(3)	62(3)	58(3)	-3(2)	14(2)	1(2)
O(38)	53(2)	68(3)	53(2)	-3(2)	11(2)	-19(2)
O(39)	68(3)	59(3)	63(3)	15(2)	8(2)	0(2)
O(40)	51(2)	54(2)	56(3)	-1(2)	5(2)	4(2)
O(41)	60(3)	53(3)	64(3)	-5(2)	13(2)	1(2)

O(42)	72(3)	42(2)	77(3)	-8(2)	19(2)	4(2)
O(43)	42(2)	51(2)	49(2)	-7(2)	7(2)	1(2)
O(44)	65(3)	70(3)	75(3)	-23(2)	14(2)	6(2)
S(1)	37(1)	38(1)	36(1)	1(1)	7(1)	-1(1)
O(51)	64(2)	26(2)	54(2)	4(2)	14(2)	-1(2)
O(52)	52(2)	53(2)	34(2)	-3(2)	8(2)	-7(2)
O(53)	44(2)	54(2)	51(2)	-4(2)	-1(2)	9(2)
O(54)	40(2)	58(2)	41(2)	2(2)	12(2)	-7(2)
S(2)	43(1)	49(1)	40(1)	-1(1)	5(1)	3(1)
O(61)	72(3)	54(3)	32(2)	-3(2)	-1(2)	7(2)
O(62)	69(3)	77(3)	41(3)	17(2)	18(2)	17(2)
O(63)	35(2)	60(3)	88(3)	-17(2)	16(2)	11(2)
O(64)	33(2)	69(3)	63(3)	-4(2)	7(2)	-10(2)
O(71)	71(10)	52(10)	33(10)	-3(9)	-2(9)	6(10)
O(72)	55(10)	80(10)	42(10)	18(10)	32(9)	20(10)
O(73)	48(10)	56(7)	92(10)	-9(10)	16(10)	11(10)
O(74)	25(9)	69(10)	64(10)	-4(10)	-6(9)	-8(10)

Table 5. Bond lengths [Å] and angles [°] for C24 H70 N6 O30 S2

O(11)-C(11')	1.394(5)	C(15')-O(12)-C(11')	116.4(4)
O(11)-C(14)	1.443(5)	C(26')-N(13)-C(13)	117.2(4)
O(12)-C(15')	1.397(5)	N(11)-C(11)-C(16)	110.3(4)
O(12)-C(11')	1.446(6)	N(11)-C(11)-C(12)	110.1(4)
O(13)-C(15)	1.428(5)	C(16)-C(11)-C(12)	109.0(4)
O(14)-C(16)	1.432(6)	C(13)-C(12)-C(11)	110.9(4)
N(11)-C(11)	1.480(6)	N(13)-C(13)-C(12)	108.7(4)
N(12)-C(12')	1.501(6)	N(13)-C(13)-C(14)	108.8(4)
N(13)-C(26')	1.271(6)	C(12)-C(13)-C(14)	111.1(4)
N(13)-C(13)	1.480(6)	O(11)-C(14)-C(15)	110.6(4)
C(11)-C(16)	1.517(7)	O(11)-C(14)-C(13)	106.1(3)
C(11)-C(12)	1.540(7)	C(15)-C(14)-C(13)	112.5(4)
C(12)-C(13)	1.518(6)	O(13)-C(15)-C(16)	111.8(4)
C(13)-C(14)	1.534(6)	O(13)-C(15)-C(14)	106.4(4)
C(14)-C(15)	1.520(6)	C(16)-C(15)-C(14)	113.0(4)
C(15)-C(16)	1.508(7)	O(14)-C(16)-C(15)	109.3(4)
C(11')-C(12')	1.525(6)	O(14)-C(16)-C(11)	109.4(4)
C(12')-C(13')	1.499(7)	C(15)-C(16)-C(11)	111.0(4)
C(13')-C(14')	1.490(7)	O(11)-C(11')-O(12)	110.6(3)
C(14')-C(15')	1.323(7)	O(11)-C(11')-C(12')	106.6(4)
C(15')-C(16')	1.463(7)	O(12)-C(11')-C(12')	110.3(4)
		C(13')-C(12')-N(12)	112.0(4)
C(16')-N(23)	1.267(6)	C(13')-C(12')-C(11')	112.3(4)
O(21)-C(21')	1.393(5)	N(12)-C(12')-C(11')	108.0(4)
O(21)-C(24)	1.457(5)	C(14')-C(13')-C(12')	108.7(4)
O(22)-C(25')	1.398(6)	C(15')-C(14')-C(13')	122.7(5)
O(22)-C(21')	1.427(5)	C(14')-C(15')-O(12)	124.2(4)
O(23)-C(25)	1.411(5)	C(14')-C(15')-C(16')	122.6(5)
O(24)-C(26)	1.443(6)	O(12)-C(15')-C(16')	113.2(4)
N(21)-C(21)	1.499(6)	N(23)-C(16')-C(15')	125.1(5)
N(22)-C(22')	1.503(6)	C(21')-O(21)-C(24)	116.0(3)
N(23)-C(23)	1.476(6)	C(25')-O(22)-C(21')	116.7(3)
C(21)-C(26)	1.525(7)	C(16')-N(23)-C(23)	115.1(4)
C(21)-C(22)	1.528(7)	N(21)-C(21)-C(26)	109.9(4)
C(22)-C(23)	1.519(7)	N(21)-C(21)-C(22)	110.4(4)
C(23)-C(24)	1.527(6)	C(26)-C(21)-C(22)	109.7(4)
C(24)-C(25)	1.535(7)	C(23)-C(22)-C(21)	109.6(4)
C(25)-C(26)	1.533(7)	N(23)-C(23)-C(22)	110.5(4)
C(21')-C(22')	1.528(6)	N(23)-C(23)-C(24)	109.7(4)
C(22')-C(23')	1.515(7)	C(22)-C(23)-C(24)	109.4(4)
C(23')-C(24')	1.505(7)	O(21)-C(24)-C(23)	107.0(4)
C(24')-C(25')	1.316(6)	O(21)-C(24)-C(25)	108.6(4)
C(25')-C(26')	1.468(7)	C(23)-C(24)-C(25)	111.9(4)
S(1)-O(52)	1.457(3)	O(23)-C(25)-C(26)	111.7(4)
S(1)-O(54)	1.462(3)	O(23)-C(25)-C(24)	107.9(4)
S(1)-O(53)	1.473(4)	C(26)-C(25)-C(24)	111.1(4)
S(1)-O(51)	1.497(4)	O(24)-C(26)-C(21)	110.7(4)
S(2)-O(72)	1.444(10)	O(24)-C(26)-C(25)	110.1(4)
S(2)-O(62)	1.449(4)	C(21)-C(26)-C(25)	110.4(4)
S(2)-O(71)	1.449(9)	O(21)-C(21')-O(22)	111.1(3)
S(2)-O(61)	1.453(4)	O(21)-C(21')-C(22')	105.9(4)
S(2)-O(63)	1.472(4)	O(22)-C(21')-C(22')	111.1(4)
S(2)-O(73)	1.475(10)	N(22)-C(22')-C(23')	110.8(4)
S(2)-O(64)	1.479(4)	N(22)-C(22')-C(21')	107.8(4)
S(2)-O(74)	1.488(10)	C(23')-C(22')-C(21')	111.9(4)
		C(24')-C(23')-C(22')	108.1(4)
C(11')-O(11)-C(14)	116.0(3)	C(25')-C(24')-C(23')	122.9(4)

C(24')-C(25')-O(22)	124.4(4)	O(72)-S(2)-O(73)	109.9(12)
C(24')-C(25')-C(26')	122.6(5)	O(62)-S(2)-O(73)	141.4(17)
O(22)-C(25')-C(26')	113.0(4)	O(71)-S(2)-O(73)	110.8(12)
N(13)-C(26')-C(25')	124.5(4)	O(61)-S(2)-O(73)	108.7(18)
O(52)-S(1)-O(54)	110.6(2)	O(63)-S(2)-O(73)	59.3(14)
O(52)-S(1)-O(53)	109.3(2)	O(72)-S(2)-O(64)	137.2(16)
O(54)-S(1)-O(53)	111.1(2)	O(62)-S(2)-O(64)	109.1(3)
O(52)-S(1)-O(51)	108.7(2)	O(71)-S(2)-O(64)	112.0(18)
O(54)-S(1)-O(51)	107.6(2)	O(61)-S(2)-O(64)	108.9(3)
O(53)-S(1)-O(51)	109.6(2)	O(63)-S(2)-O(64)	108.8(3)
O(72)-S(2)-O(62)	57.1(13)	O(73)-S(2)-O(64)	52.9(14)
O(72)-S(2)-O(71)	110.8(13)	O(72)-S(2)-O(74)	109.4(12)
O(62)-S(2)-O(71)	107.7(18)	O(62)-S(2)-O(74)	56.4(14)
O(72)-S(2)-O(61)	113.9(17)	O(71)-S(2)-O(74)	109.0(13)
O(62)-S(2)-O(61)	109.6(3)	O(61)-S(2)-O(74)	107.9(17)
O(71)-S(2)-O(61)	3.1(19)	O(63)-S(2)-O(74)	141.4(16)
O(72)-S(2)-O(63)	54.7(14)	O(73)-S(2)-O(74)	106.8(12)
O(62)-S(2)-O(63)	109.8(3)	O(64)-S(2)-O(74)	56.1(14)
O(71)-S(2)-O(63)	109.5(18)		
O(61)-S(2)-O(63)	110.7(3)		

Table 6. Torsion angles [°] for C24 H70 N6 O30 S2.

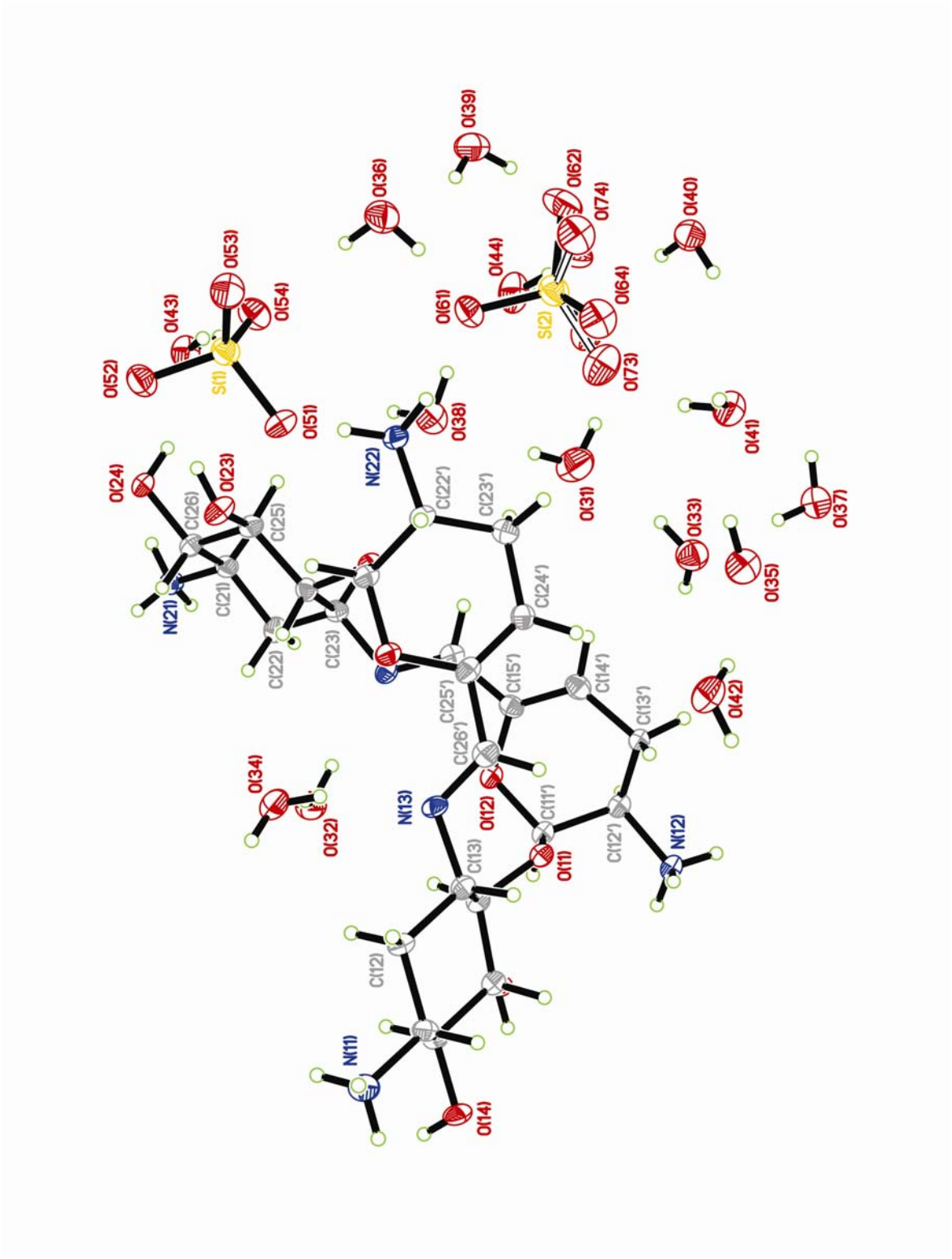
N(11)-C(11)-C(12)-C(13) 178.7(4)	C(26)-C(21)-C(22)-C(23) -62.3(5)
C(16)-C(11)-C(12)-C(13) -60.2(5)	C(16')-N(23)-C(23)-C(22) 149.4(4)
C(26')-N(13)-C(13)-C(12) 148.6(4)	C(16')-N(23)-C(23)-C(24) -89.8(5)
C(26')-N(13)-C(13)-C(14) -90.3(5)	C(21)-C(22)-C(23)-N(23) -178.6(4)
C(11)-C(12)-C(13)-N(13) 175.8(4)	C(21)-C(22)-C(23)-C(24) 60.5(5)
C(11)-C(12)-C(13)-C(14) 56.1(5)	C(21')-O(21)-C(24)-C(23) -149.5(4)
C(11')-O(11)-C(14)-C(15) 85.3(4)	C(21')-O(21)-C(24)-C(25) 89.6(4)
C(11')-O(11)-C(14)-C(13) -152.5(4)	N(23)-C(23)-C(24)-O(21) 63.2(5)
N(13)-C(13)-C(14)-O(11) 68.7(4)	C(22)-C(23)-C(24)-O(21) -175.3(4)
C(12)-C(13)-C(14)-O(11) -171.7(4)	N(23)-C(23)-C(24)-C(25) -177.9(4)
N(13)-C(13)-C(14)-C(15) -170.2(4)	C(22)-C(23)-C(24)-C(25) -56.5(5)
C(12)-C(13)-C(14)-C(15) -50.6(5)	O(21)-C(24)-C(25)-O(23) -65.8(5)
O(11)-C(14)-C(15)-O(13) -68.4(4)	C(23)-C(24)-C(25)-O(23) 176.4(4)
C(13)-C(14)-C(15)-O(13) 173.2(4)	O(21)-C(24)-C(25)-C(26) 171.4(4)
O(11)-C(14)-C(15)-C(16) 168.5(4)	C(23)-C(24)-C(25)-C(26) 53.6(5)
C(13)-C(14)-C(15)-C(16) 50.1(5)	N(21)-C(21)-C(26)-O(24) -57.4(5)
O(13)-C(15)-C(16)-O(14) 64.5(5)	C(22)-C(21)-C(26)-O(24) -179.0(4)
C(14)-C(15)-C(16)-O(14) -175.5(4)	N(21)-C(21)-C(26)-C(25) -179.7(4)
O(13)-C(15)-C(16)-C(11) -174.7(4)	C(22)-C(21)-C(26)-C(25) 58.7(5)
C(14)-C(15)-C(16)-C(11) -54.7(5)	O(23)-C(25)-C(26)-O(24) 62.6(5)
N(11)-C(11)-C(16)-O(14) -59.4(5)	C(24)-C(25)-C(26)-O(24) -176.8(4)
C(12)-C(11)-C(16)-O(14) 179.6(4)	O(23)-C(25)-C(26)-C(21) -174.8(4)
N(11)-C(11)-C(16)-C(15) 179.8(4)	C(24)-C(25)-C(26)-C(21) -54.3(5)
C(12)-C(11)-C(16)-C(15) 58.8(5)	C(24)-O(21)-C(21')-O(22) 82.1(4)
C(14)-O(11)-C(11')-O(12) 74.7(5)	C(24)-O(21)-C(21')-C(22') -157.2(3)
C(14)-O(11)-C(11')-C(12') -165.4(4)	C(25')-O(22)-C(21')-O(21) 80.4(4)
C(15')-O(12)-C(11')-O(11) 79.8(5)	C(25')-O(22)-C(21')-C(22') -37.2(5)
C(15')-O(12)-C(11')-C(12') -37.8(5)	O(21)-C(21')-C(22')-N(22) 59.1(4)
O(11)-C(11')-C(12')-C(13') -62.1(5)	O(22)-C(21')-C(22')-N(22) 179.8(3)
O(12)-C(11')-C(12')-C(13') 58.1(5)	O(21)-C(21')-C(22')-C(23') -63.0(5)
O(11)-C(11')-C(12')-N(12) 62.0(5)	O(22)-C(21')-C(22')-C(23') 57.8(5)
O(12)-C(11')-C(12')-N(12) -177.9(3)	N(22)-C(22')-C(23')-C(24') -167.6(4)
N(12)-C(12')-C(13')-C(14') -169.5(4)	C(21')-C(22')-C(23')-C(24') -47.3(5)
C(11')-C(12')-C(13')-C(14') -47.7(5)	C(22')-C(23')-C(24')-C(25') 20.7(6)
C(12')-C(13')-C(14')-C(15') 20.6(7)	C(23')-C(24')-C(25')-O(22) -1.2(7)
C(13')-C(14')-C(15')-O(12) -1.6(8)	C(23')-C(24')-C(25')-C(26') 176.0(4)
C(13')-C(14')-C(15')-C(16') 178.5(4)	C(21')-O(22)-C(25')-C(24') 9.8(6)
C(11')-O(12)-C(15')-C(14') 10.9(6)	C(21')-O(22)-C(25')-C(26') -167.5(4)
C(11')-O(12)-C(15')-C(16') -169.2(4)	C(13)-N(13)-C(26')-C(25') 176.2(4)
C(14')-C(15')-C(16')-N(23) -167.3(5)	C(24')-C(25')-C(26')-N(13) -170.1(4)
O(12)-C(15')-C(16')-N(23) 12.8(7)	O(22)-C(25')-C(26')-N(13) 7.3(6)
C(15')-C(16')-N(23)-C(23) 177.1(4)	
N(21)-C(21)-C(22)-C(23) 176.5(4)	

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C24 H70 N6 O30 S2.

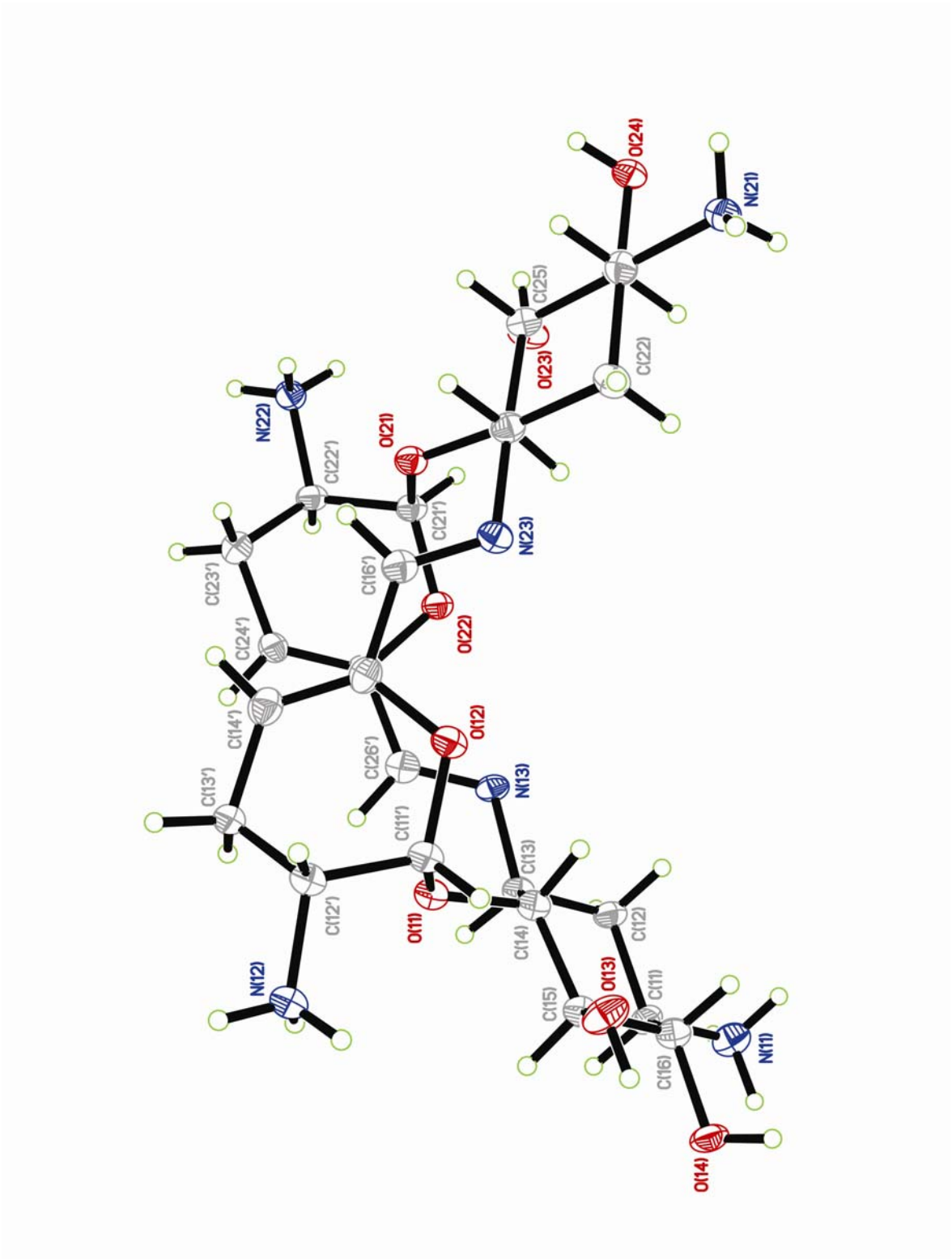
D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(13)-H(13D)	O(24)#1	0.84	2.03	2.774(4)	147.3
O(14)-H(14C)	O(52)#2	0.84	1.88	2.699(4)	162.9
N(11)-H(11A)	O(37)#3	0.91	2.04	2.832(5)	145.3
N(11)-H(11B)	O(43)#2	0.91	2.11	2.863(5)	140
N(11)-H(11B)	O(24)#2	0.91	2.56	3.171(5)	125.5
N(11)-H(11C)	O(35)#4	0.91	1.98	2.869(6)	164.4
N(12)-H(12A)	O(36)#5	0.91	2	2.889(6)	163.8
N(12)-H(12B)	O(54)#5	0.91	1.92	2.774(5)	155
N(12)-H(12C)	O(39)#6	0.91	2.04	2.854(6)	148.4
O(23)-H(23D)	O(43)	0.84	2.11	2.902(5)	156.4
O(23)-H(23D)	O(14)#7	0.84	2.6	3.047(4)	114.4
O(24)-H(24C)	O(52)#8	0.84	1.96	2.734(5)	153.6
N(21)-H(21A)	O(72)#9	0.91	1.78	2.59(3)	146.5
N(21)-H(21A)	O(62)#9	0.91	1.88	2.773(5)	168.5
N(21)-H(21B)	O(40)#9	0.91	1.86	2.766(5)	174.1
N(21)-H(21C)	O(14)#10	0.91	2.07	2.962(5)	167.5
N(22)-H(22A)	O(38)	0.91	1.96	2.850(5)	165.2
N(22)-H(22B)	O(61)	0.91	1.8	2.700(6)	168.3
N(22)-H(22B)	O(71)	0.91	1.81	2.71(4)	167.5
N(22)-H(22C)	O(51)	0.91	2.21	2.900(5)	132.6
N(22)-H(22C)	O(54)	0.91	2.51	3.233(5)	137.3
O(31)-H(31A)	O(38)	0.874(7)	2.104(14)	2.970(6)	171(6)
O(31)-H(31B)	O(64)#8	0.873(7)	2.03(3)	2.841(6)	155(6)
O(31)-H(31B)	O(73)#8	0.873(7)	2.10(6)	2.80(3)	136(6)
O(32)-H(32A)	N(23)	0.874(7)	2.024(17)	2.853(5)	158(4)
O(32)-H(32B)	O(34)	0.875(7)	1.921(13)	2.782(5)	168(5)
O(33)-H(33A)	O(31)	0.874(7)	1.96(3)	2.774(6)	154(6)
O(33)-H(33B)	O(42)#8	0.873(7)	1.946(11)	2.801(6)	166(3)
O(34)-H(34A)	O(41)#4	0.873(7)	1.971(11)	2.826(6)	166(3)
O(34)-H(34B)	N(13)	0.874(7)	2.02(3)	2.854(5)	160(7)
O(35)-H(35A)	O(33)	0.873(7)	1.949(18)	2.808(6)	168(7)
O(35)-H(35B)	O(41)	0.873(7)	2.04(2)	2.887(6)	165(7)
O(36)-H(36A)	O(53)#8	0.873(7)	1.958(17)	2.816(5)	167(6)
O(36)-H(36B)	O(44)	0.874(7)	1.894(11)	2.720(6)	157(2)
O(37)-H(37A)	O(33)	0.873(7)	1.963(10)	2.835(6)	177(5)
O(37)-H(37B)	O(32)#11	0.874(7)	1.875(11)	2.744(5)	173(6)
O(38)-H(38A)	O(51)#8	0.874(7)	1.891(12)	2.757(5)	171(6)
O(38)-H(38B)	O(44)	0.874(7)	1.886(19)	2.722(6)	159(5)
O(39)-H(39A)	O(36)	0.873(7)	2.12(2)	2.946(6)	157(5)
O(39)-H(39B)	O(62)#8	0.874(7)	1.95(3)	2.778(6)	157(7)
O(39)-H(39B)	O(74)#8	0.874(7)	1.98(5)	2.76(4)	148(5)
O(40)-H(40A)	O(74)#8	0.873(7)	1.84(5)	2.61(3)	146(5)
O(40)-H(40A)	O(64)#8	0.873(7)	1.94(2)	2.773(5)	159(5)
O(40)-H(40B)	O(34)#11	0.873(7)	1.90(4)	2.696(5)	151(7)
O(41)-H(41A)	O(73)	0.873(7)	2.20(4)	2.80(3)	125(3)
O(41)-H(41A)	O(32)#12	0.873(7)	2.38(4)	2.801(5)	110(3)
O(41)-H(41B)	O(63)	0.873(7)	2.24(2)	2.801(6)	121(2)
O(42)-H(42A)	O(35)	0.873(7)	2.18(2)	3.006(6)	158(5)
O(42)-H(42B)	O(53)#13	0.873(7)	2.12(2)	2.959(6)	162(7)
O(43)-H(43A)	O(54)	0.873(7)	1.850(13)	2.718(4)	172(6)
O(43)-H(43B)	O(53)#8	0.873(7)	1.988(13)	2.853(5)	171(6)
O(44)-H(44A)	O(72)	0.871(6)	1.72(4)	2.49(3)	145(4)
O(44)-H(44A)	O(63)	0.871(6)	2.07(6)	2.653(6)	124(6)
O(44)-H(44B)	O(74)#8	0.871(6)	1.92(5)	2.72(4)	151(5)
O(44)-H(44B)	O(64)#8	0.871(6)	1.93(3)	2.762(6)	160(7)

Symmetry transformations used to generate equivalent atoms:

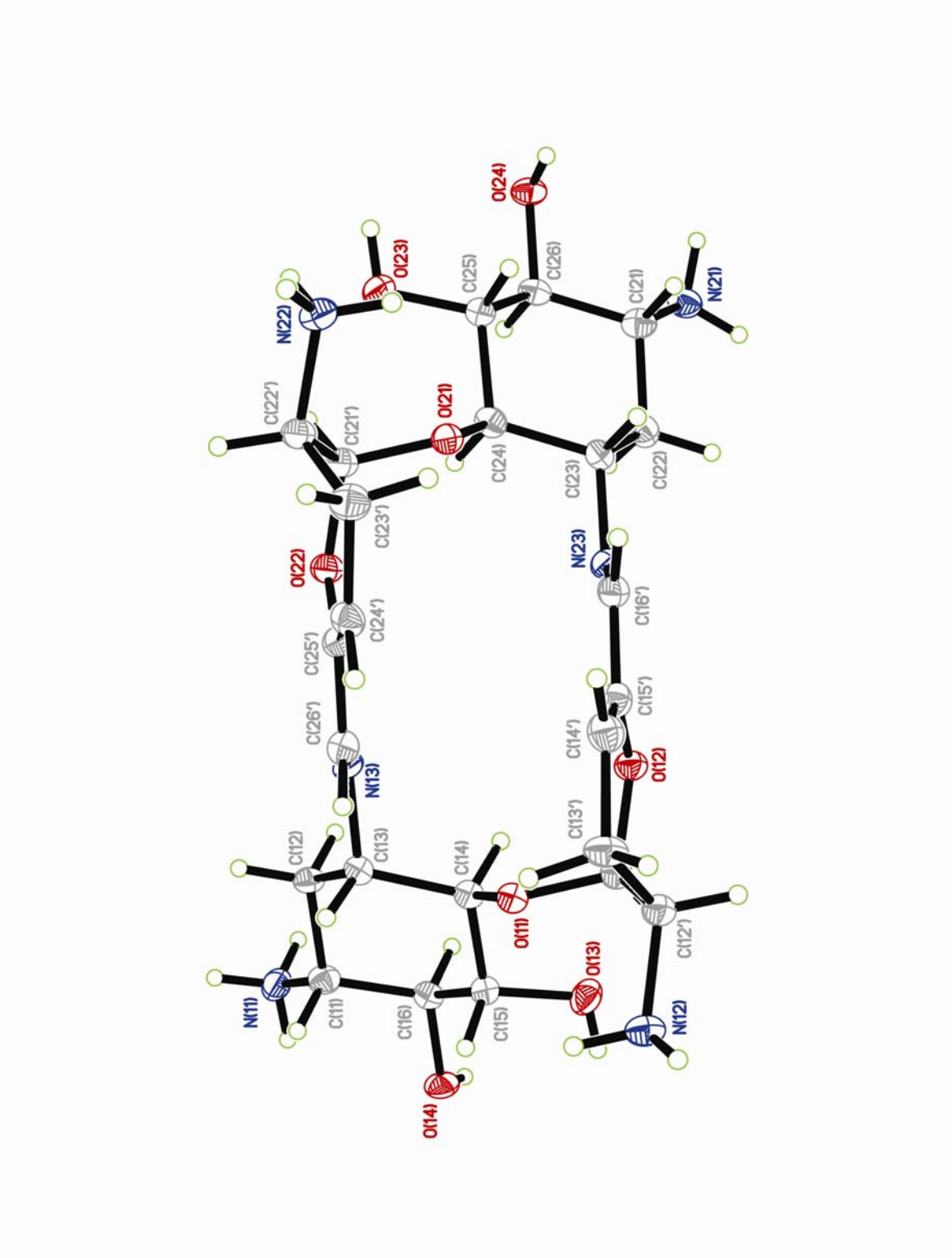
#1 -x,y+1/2,-z	#2 -x+1,y+1/2,-z	#3 x+1,y,z-1
#4 x,y,z-1	#5 -x+1,y+1/2,-z+1	#6 -x,y+1/2,-z+1
#7 -x+1,y-1/2,-z	#8 x-1,y,z	#9 x-1,y,z-1
#10 -x,y-1/2,-z	#11 x,y,z+1	#12 x+1,y,z+1
#13 -x+2,y+1/2,-z+1		



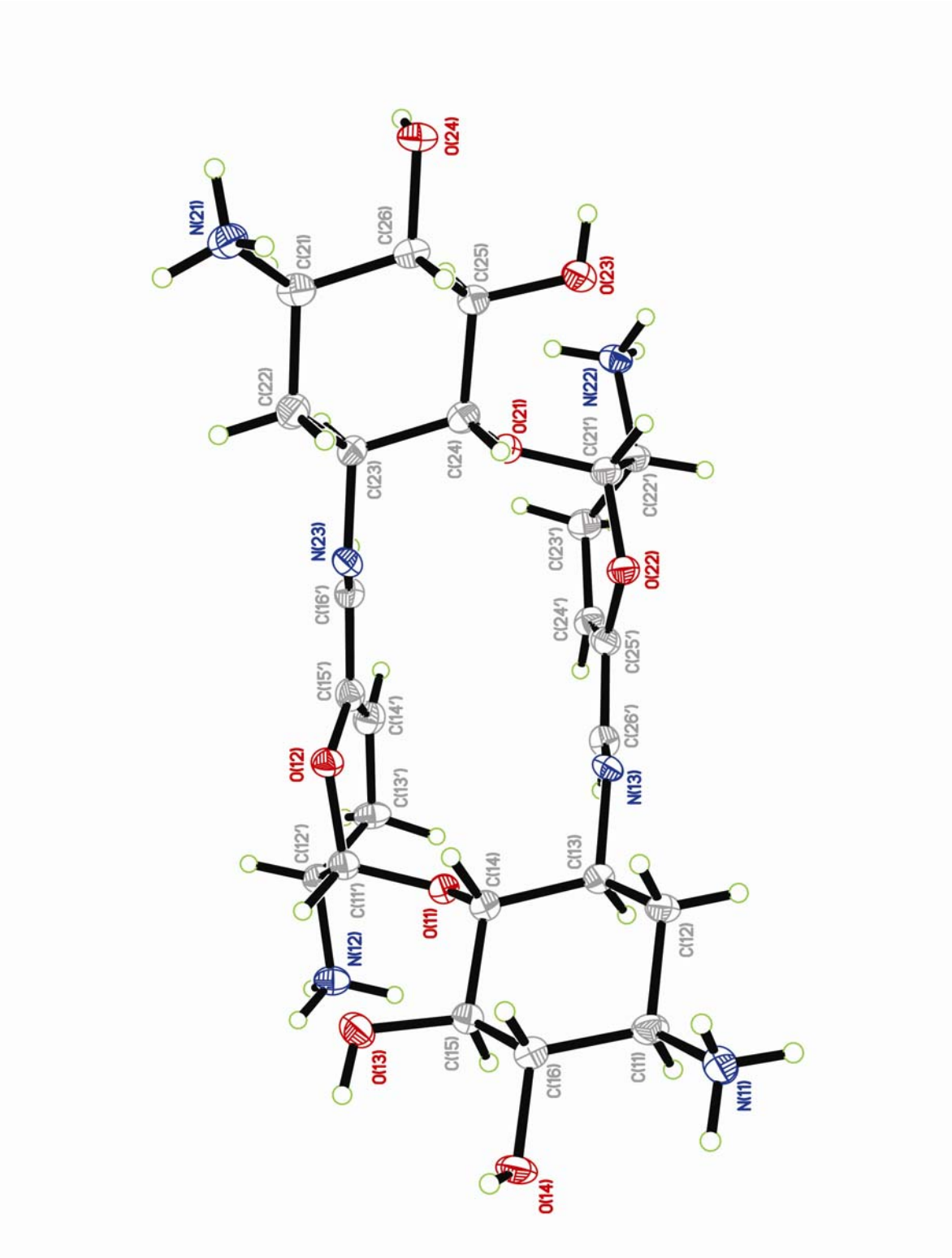
ORTEP view of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP side view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP top view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP bottom view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: bent66

Bond precision: C-C = 0.0069 A Wavelength=1.54178
Cell: a=6.8516(4) b=26.1435(15) c=12.6653(7)
alpha=90 beta=102.975(3) gamma=90
Temperature: 200 K

	Calculated	Reported
Volume	2210.8(2)	2210.7(2)
Space group	P 21	P21
Hall group	P 2yb	P 2yb
Moiety formula	C24 H42 N6 O8, 2(O4 S), 14(H2 O)	C24 H42 N6 O8, 2(O4 S), 14(H2 O)
Sum formula	C24 H70 N6 O30 S2	C24 H70 N6 O30 S2
Mr	987.00	986.98
Dx,g cm-3	1.483	1.483
Z	2	2
Mu (mm-1)	2.018	2.018
F000	1056.0	1056.0
F000'	1061.39	
h,k,lmax	7,27,13	7,27,13
Nref	2714[5282]	5428
Tmin,Tmax	0.804,0.941	0.663,0.941
Tmin'	0.493	

Correction method= MULTI-SCAN
Data completeness= 2.00/1.03 Theta(max)= 53.690
R(reflections)= 0.0437(4867) wR2(reflections)= 0.1060(5428)
S = 1.077 Npar= 689

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5227

Author Response: Low diffraction was observed for this crystal and was especially low for high angles. Many solvent systems were tested for recrystallization. The best crystal was chosen and its size was in the limits of the diffractometer. X-ray measurements were acquired at 200K with optimized radiation exposure time and intensity. The final structure was satisfactory for confirming the desired chemical information with R1 = 0.0437 and wR2=0.1060.

Alert level C

REFNR01_ALERT_3_C Ratio of reflections to parameters is < 8 for a
non-centrosymmetric structure, where ZMAX < 18
sine(theta)/lambda 0.5227
Proportion of unique data used 1.0000
Ratio reflections to parameters 7.8781

Author Response: See response for THETM01 Alert 3 A.

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) 7.88

Author Response: See response for THETM01 Alert 3 A.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0069 Ang

Author Response: See response for THETM01 Alert 3 A.

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 53.69
From the CIF: _reflns_number_total 5428
Count of symmetry unique reflns 2714
Completeness (_total/calc) 200.00%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2714
Fraction of Friedel pairs measured 1.000
Are heavy atom types Z>Si present yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 51
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 20
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 17 Perc.
PLAT791_ALERT_4_G Note: The Model has Chirality at C11 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C11' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C12' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C13 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C14 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C15 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C16 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C21 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C21' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C22' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C23 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C24 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C25 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C26 (Verify) S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 572

1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
20 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
16 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

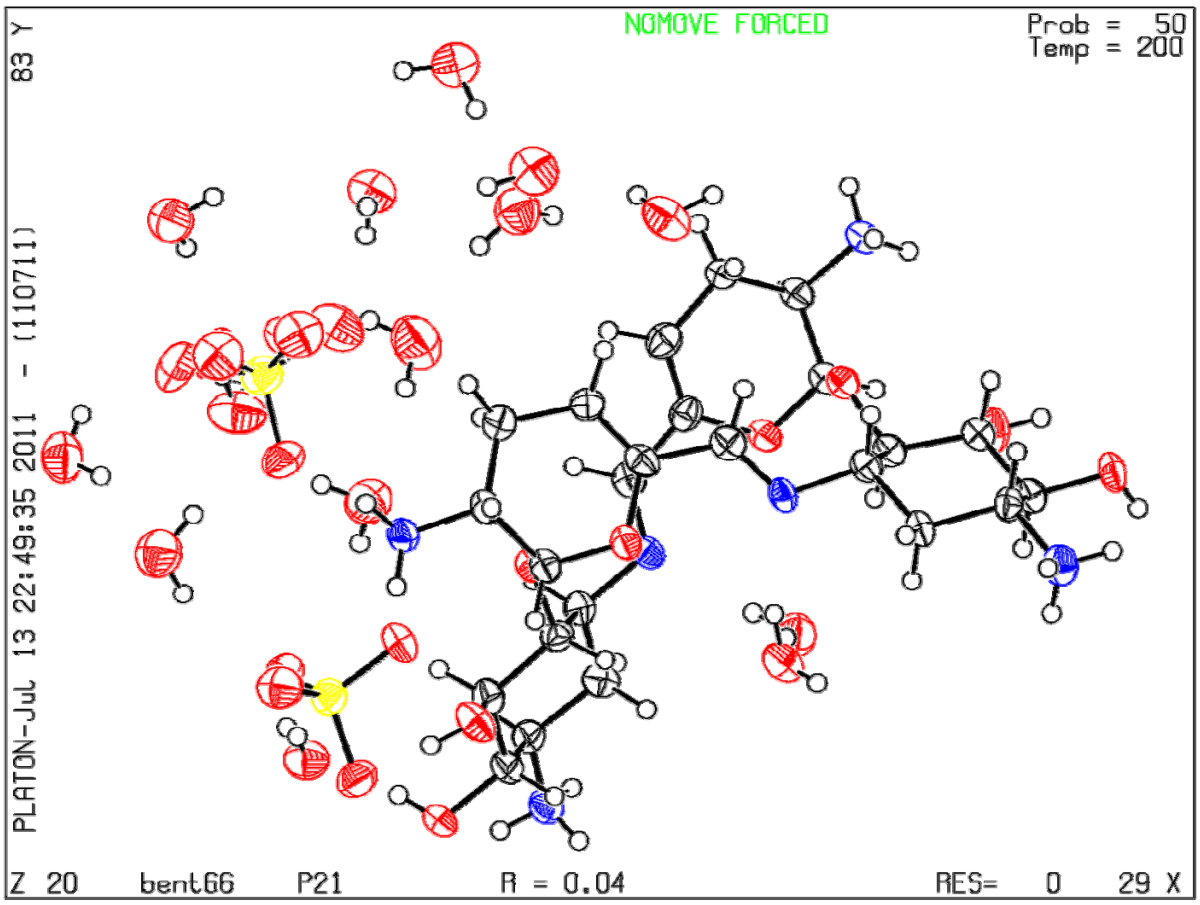
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/07/2011; check.def file version of 04/07/2011

Datablock bent66 - ellipsoid plot



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Université de Montréal

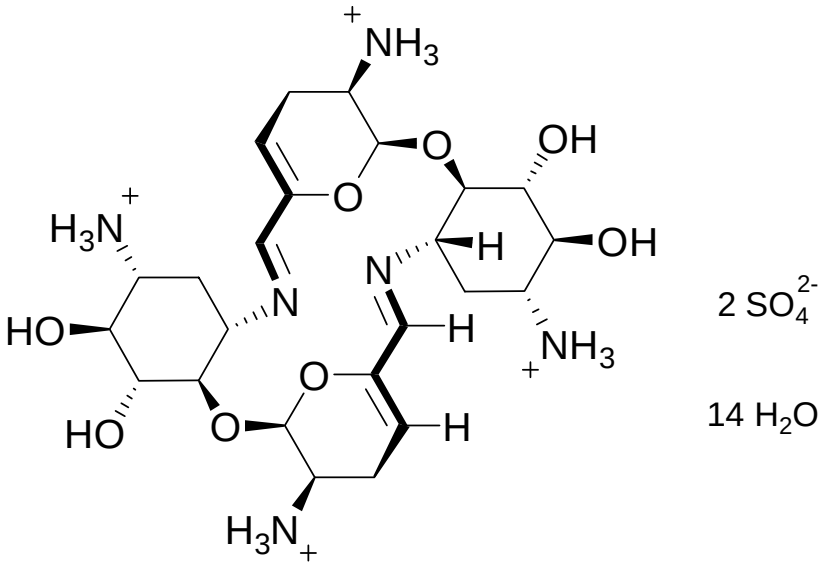
CRYSTAL AND MOLECULAR STRUCTURE OF

C24 H42 N6 O8 • 2(S O4) • 14(H2 O) COMPOUND (bent68)

Equipe Hanessian

Département de chimie, Université de Montréal,

C.P. 6128, Succ. Centre-Ville, Montréal, Québec, H3C 3J7 (Canada)



2 SO_4^{2-}

14 H_2O

Measured at 170K with phase transition to orthorhombic crystal system
(See monoclinic crystal system measured at 200K)

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C24 H70 N6 O30 S2.

Identification code	bent68
Empirical formula (ions and solvents)	C24 H42 N6 O8 • 2(S O4) • 14(H2 O)
Empirical formula sum	C24 H70 N6 O30 S2
Formula weight	986.98
Temperature	170K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	C2221
Unit cell dimensions	a = 6.74530(10) Å α = 90° b = 25.6806(5) Å β = 90° c = 25.6822(5) Å γ = 90°
Volume	4448.76(14)Å^3
Z	4
Density (calculated)	1.474 g/cm^3
Absorption coefficient	2.005 mm^{-1}
F(000)	2112
Crystal size	0.36 x 0.09 x 0.02 mm
Theta range for data collection	3.44 to 72.54°
Index ranges	$-8 \le h \le 8$, $-28 \le k \le 31$, $-31 \le \ell \le 31$
Reflections collected	29758
Independent reflections	4389 [R_{int} = 0.036]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9607 and 0.7782
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4389 / 34 / 364
Goodness-of-fit on F^2	1.073
Final R indices [I>2sigma(I)]	R_1 = 0.0335, wR_2 = 0.1016
R indices (all data)	R_1 = 0.0350, wR_2 = 0.1030

Absolute structure parameter	0.017(16)
Largest diff. peak and hole	0.258 and -0.286 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for C24 H70 N6 O30 S2.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	x	y	z	U_{eq}
S(1)	1	5296(1)	997(1)	5321(1)	29(1)
O(1)	1	-2483(2)	1078(1)	3129(1)	23(1)
O(2)	1	162(2)	971(1)	3706(1)	22(1)
O(3)	1	-660(2)	1723(1)	4510(1)	32(1)
O(4)	1	2921(2)	2227(1)	4919(1)	27(1)
O(5)	1	5023(3)	881(1)	4764(1)	39(1)
O(6)	1	5501(3)	1561(1)	5397(1)	38(1)
O(7)	1	3579(3)	805(1)	5617(1)	44(1)
O(8)	1	7119(3)	734(1)	5502(1)	47(1)
N(1)	1	5823(3)	2521(1)	4167(1)	29(1)
N(2)	1	2703(2)	1336(1)	2906(1)	22(1)
N(3)	1	-1836(3)	284(1)	4329(1)	31(1)
C(1)	1	4548(3)	2049(1)	4094(1)	23(1)
C(2)	1	4202(3)	1945(1)	3517(1)	24(1)
C(3)	1	3032(3)	1441(1)	3458(1)	21(1)
C(4)	1	1025(3)	1481(1)	3738(1)	21(1)
C(5)	1	1274(3)	1634(1)	4309(1)	24(1)
C(6)	1	2584(3)	2119(1)	4380(1)	24(1)
C(1')	1	-1896(3)	948(1)	3648(1)	21(1)
C(2')	1	-2535(3)	397(1)	3793(1)	25(1)
C(3')	1	-1732(3)	-5(1)	3416(1)	27(1)
C(4')	1	-2133(3)	179(1)	2874(1)	25(1)
C(5')	1	-2430(3)	683(1)	2766(1)	22(1)
C(6')	1	-2756(3)	858(1)	2230(1)	23(1)
O(9)	1	6929(4)	1776(1)	6427(1)	63(1)
O(10)	1	8460(3)	2705(1)	3288(1)	42(1)
O(11)	1	162(3)	1433(1)	5590(1)	40(1)
O(12A)	0.60	2385(9)	197(2)	4308(2)	52(1)
O(12B)	0.40	1876(15)	179(4)	4551(5)	79(3)
O(13)	1	10441(4)	1582(1)	6969(1)	65(1)
O(14)	1	2670(4)	701(1)	6723(1)	72(1)
O(15)	0.50	5554(12)	1004(3)	7338(3)	99(2)
O(16)	1	0	2073(1)	2500	34(1)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C24 H70 N6 O30 S2.

	Occ.	x	y	z	U_{eq}
H(3)	1	-635	1703	4836	48
H(4)	1	3568	1981	5052	41
H(1A)	1	6340	2520	4494	43
H(1B)	1	5078	2813	4121	43
H(1C)	1	6825	2517	3930	43
H(3A)	1	-2194	-46	4419	46
H(3B)	1	-2394	514	4555	46
H(3C)	1	-493	314	4342	46
H(1)	1	5251	1743	4247	27
H(2A)	1	3455	2237	3360	28
H(2B)	1	5490	1914	3334	28
H(3D)	1	3811	1148	3613	25
H(4A)	1	158	1739	3556	26
H(5)	1	1887	1337	4502	28
H(6)	1	1877	2424	4223	28
H(1')	1	-2522	1200	3895	26
H(2')	1	-4017	380	3788	30
H(3'1)	1	-289	-50	3469	32
H(3'2)	1	-2387	-345	3476	32
H(4')	1	-2178	-69	2599	31
H(6')	1	-3020	604	1971	28
H(9A)	1	6650(70)	1654(15)	6119(8)	94
H(9B)	0.50	6510(130)	1524(19)	6627(16)	94
H(9C)	0.50	5960(70)	1990(30)	6500(20)	94
H(10A)	1	8890(50)	2485(10)	3055(10)	63
H(10B)	1	7490(40)	2859(12)	3136(11)	63
H(11A)	1	-780(30)	1200(10)	5605(14)	60
H(11B)	1	1210(30)	1248(11)	5656(14)	60
H(12A)	0.60	3150(90)	390(20)	4490(30)	78
H(12B)	0.60	2580(110)	-121(8)	4390(30)	78
H(12C)	0.40	2890(100)	380(30)	4600(70)	118
H(12D)	0.40	2280(160)	-138(14)	4550(60)	118
H(13A)	0.50	11120(80)	1320(20)	6850(40)	97
H(13B)	0.50	9240(40)	1520(30)	6860(30)	97
H(13C)	0.50	10480(100)	1640(20)	7305(5)	97
H(13D)	0.50	9950(150)	1265(16)	6948(19)	97
H(14A)	1	3130(70)	804(16)	6421(9)	109
H(14B)	0.50	3530(80)	820(30)	6939(16)	109
H(14C)	0.50	2760(170)	365(5)	6690(30)	109
H(15A)	0.50	5300(200)	1090(40)	7657(17)	148
H(15B)	0.50	6150(110)	1260(30)	7190(20)	148
H(16A)	1	1030(30)	1878(10)	2572(13)	51

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C24 H70 N6 O30 S2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
S(1)	25(1)	29(1)	35(1)	2(1)	-3(1)	1(1)
O(1)	24(1)	24(1)	19(1)	2(1)	-3(1)	1(1)
O(2)	19(1)	23(1)	24(1)	0(1)	-1(1)	0(1)
O(3)	23(1)	48(1)	25(1)	-7(1)	5(1)	-1(1)
O(4)	30(1)	32(1)	20(1)	-6(1)	-2(1)	4(1)
O(5)	40(1)	42(1)	36(1)	-4(1)	0(1)	2(1)
O(6)	40(1)	30(1)	45(1)	-1(1)	-11(1)	3(1)
O(7)	41(1)	44(1)	47(1)	3(1)	9(1)	-5(1)
O(8)	35(1)	34(1)	73(1)	11(1)	-17(1)	2(1)
N(1)	32(1)	31(1)	24(1)	-4(1)	0(1)	-5(1)
N(2)	19(1)	29(1)	18(1)	-3(1)	-1(1)	-1(1)
N(3)	44(1)	30(1)	19(1)	5(1)	1(1)	-1(1)
C(1)	22(1)	24(1)	22(1)	-2(1)	-2(1)	-1(1)
C(2)	22(1)	29(1)	20(1)	-1(1)	0(1)	-1(1)
C(3)	19(1)	26(1)	18(1)	-2(1)	0(1)	0(1)
C(4)	19(1)	23(1)	21(1)	-1(1)	0(1)	0(1)
C(5)	22(1)	30(1)	19(1)	-2(1)	2(1)	4(1)
C(6)	26(1)	28(1)	18(1)	-3(1)	-2(1)	5(1)
C(1')	20(1)	27(1)	17(1)	0(1)	-1(1)	2(1)
C(2')	25(1)	30(1)	20(1)	5(1)	0(1)	-2(1)
C(3')	33(1)	24(1)	25(1)	2(1)	-1(1)	0(1)
C(4')	27(1)	27(1)	22(1)	0(1)	0(1)	-1(1)
C(5')	19(1)	27(1)	20(1)	-1(1)	-1(1)	-3(1)
C(6')	20(1)	28(1)	21(1)	0(1)	-2(1)	-2(1)
O(9)	55(1)	70(1)	63(1)	-22(1)	-16(1)	14(1)
O(10)	43(1)	43(1)	41(1)	-2(1)	7(1)	-3(1)
O(11)	32(1)	42(1)	47(1)	-1(1)	2(1)	-4(1)
O(12A)	41(3)	36(2)	80(3)	4(2)	-28(2)	3(2)
O(12B)	56(6)	53(4)	128(9)	-20(6)	-49(6)	13(4)
O(13)	59(1)	86(2)	50(1)	3(1)	-1(1)	-5(1)
O(14)	74(2)	86(2)	57(1)	9(1)	1(1)	-11(1)
O(15)	108(6)	93(4)	95(5)	17(3)	-28(4)	-11(4)
O(16)	38(1)	31(1)	32(1)	0	-6(1)	0

Table 5. Bond lengths [Å] and angles [°] for C24 H70 N6 O30 S2

S(1)-O(6)	1.4661(15)	O(5)-S(1)-O(8)	108.41(11)
S(1)-O(7)	1.4700(18)	C(5')-O(1)-C(1')	116.77(14)
S(1)-O(5)	1.4738(16)	C(1')-O(2)-C(4)	116.56(14)
S(1)-O(8)	1.4785(17)	C(6')#1-N(2)-C(3)	116.06(16)
O(1)-C(5')	1.379(2)	N(1)-C(1)-C(2)	110.61(15)
O(1)-C(1')	1.431(2)	N(1)-C(1)-C(6)	110.07(15)
O(2)-C(1')	1.397(2)	C(2)-C(1)-C(6)	110.84(15)
O(2)-C(4)	1.435(2)	C(3)-C(2)-C(1)	108.95(15)
O(3)-C(5)	1.421(2)	N(2)-C(3)-C(2)	109.35(14)
O(4)-C(6)	1.430(2)	N(2)-C(3)-C(4)	109.42(15)
N(1)-C(1)	1.498(2)	C(2)-C(3)-C(4)	110.74(15)
N(2)-C(6')#1	1.275(2)	O(2)-C(4)-C(5)	109.54(15)
N(2)-C(3)	1.461(2)	O(2)-C(4)-C(3)	105.69(14)
N(3)-C(2')	1.485(2)	C(5)-C(4)-C(3)	111.65(15)
C(1)-C(2)	1.524(2)	O(3)-C(5)-C(4)	106.77(15)
C(1)-C(6)	1.525(3)	O(3)-C(5)-C(6)	110.78(15)
C(2)-C(3)	1.524(2)	C(4)-C(5)-C(6)	112.63(15)
C(3)-C(4)	1.536(2)	O(4)-C(6)-C(1)	110.51(16)
C(4)-C(5)	1.529(2)	O(4)-C(6)-C(5)	111.17(15)
C(5)-C(6)	1.538(3)	C(1)-C(6)-C(5)	110.32(15)
C(1')-C(2')	1.526(3)	O(2)-C(1')-O(1)	111.41(14)
C(2')-C(3')	1.515(3)	O(2)-C(1')-C(2')	107.07(15)
C(3')-C(4')	1.495(3)	O(1)-C(1')-C(2')	111.44(14)
C(4')-C(5')	1.339(3)	N(3)-C(2')-C(3')	110.21(16)
C(5')-C(6')	1.464(2)	N(3)-C(2')-C(1')	108.53(15)
C(6')-N(2)#1	1.275(2)	C(3')-C(2')-C(1')	112.07(16)
		C(4')-C(3')-C(2')	108.34(16)
O(6)-S(1)-O(7)	109.72(11)	C(5')-C(4')-C(3')	121.71(17)
O(6)-S(1)-O(5)	109.87(10)	C(4')-C(5')-O(1)	125.17(17)
O(7)-S(1)-O(5)	109.62(10)	C(4')-C(5')-C(6')	121.03(16)
O(6)-S(1)-O(8)	109.37(10)	O(1)-C(5')-C(6')	113.80(15)
O(7)-S(1)-O(8)	109.82(11)	N(2)#1-C(6')-C(5')	123.35(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2 #2 -x+1,y,-z+3/2

Table 6. Torsion angles [°] for C24 H70 N6 O30 S2.

N(1)-C(1)-C(2)-C(3)	175.86(16)	C(4)-C(5)-C(6)-O(4)	-175.17(15)
C(6)-C(1)-C(2)-C(3)	-61.77(19)	O(3)-C(5)-C(6)-C(1)	-171.72(15)
C(6')#1-N(2)-C(3)-C(2)	143.78(17)	C(4)-C(5)-C(6)-C(1)	-52.2(2)
C(6')#1-N(2)-C(3)-C(4)	-94.76(19)	C(4)-O(2)-C(1')-O(1)	75.33(18)
C(1)-C(2)-C(3)-N(2)	-179.67(15)	C(4)-O(2)-C(1')-C(2')	-162.59(14)
C(1)-C(2)-C(3)-C(4)	59.68(19)	C(5')-O(1)-C(1')-O(2)	83.98(19)
C(1')-O(2)-C(4)-C(5)	94.96(17)	C(5')-O(1)-C(1')-C(2')	-35.5(2)
C(1')-O(2)-C(4)-C(3)	-144.61(15)	O(2)-C(1')-C(2')-N(3)	56.54(19)
N(2)-C(3)-C(4)-O(2)	65.59(17)	O(1)-C(1')-C(2')-N(3)	178.60(15)
C(2)-C(3)-C(4)-O(2)	-173.80(14)	O(2)-C(1')-C(2')-C(3')	-65.40(19)
N(2)-C(3)-C(4)-C(5)	-175.37(15)	O(1)-C(1')-C(2')-C(3')	56.7(2)
C(2)-C(3)-C(4)-C(5)	-54.8(2)	N(3)-C(2')-C(3')-C(4')	-169.10(16)
O(2)-C(4)-C(5)-O(3)	-70.46(19)	C(1')-C(2')-C(3')-C(4')	-48.1(2)
C(3)-C(4)-C(5)-O(3)	172.82(15)	C(2')-C(3')-C(4')-C(5')	22.6(3)
O(2)-C(4)-C(5)-C(6)	167.74(14)	C(3')-C(4')-C(5')-O(1)	-2.7(3)
C(3)-C(4)-C(5)-C(6)	51.0(2)	C(3')-C(4')-C(5')-C(6')	177.97(18)
N(1)-C(1)-C(6)-O(4)	-56.2(2)	C(1')-O(1)-C(5')-C(4')	9.4(3)
C(2)-C(1)-C(6)-O(4)	-178.93(15)	C(1')-O(1)-C(5')-C(6')	-171.24(15)
N(1)-C(1)-C(6)-C(5)	-179.59(15)	C(4')-C(5')-C(6')-N(2)#1	-167.4(2)
C(2)-C(1)-C(6)-C(5)	57.72(19)	O(1)-C(5')-C(6')-N(2)#1	13.2(3)
O(3)-C(5)-C(6)-O(4)	65.32(19)		

Symmetry transformations used to generate equivalent atoms:

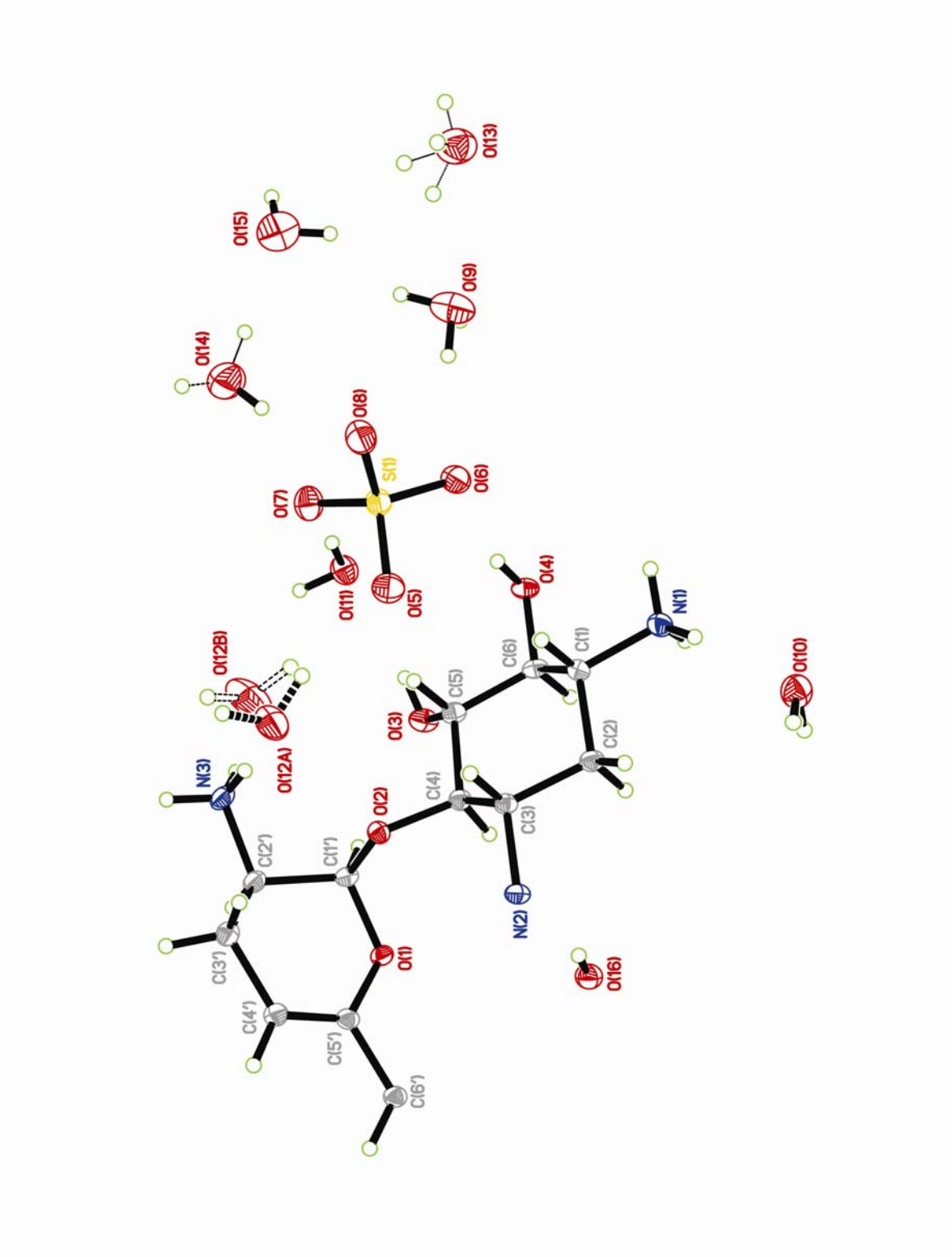
#1 -x,y,-z+1/2 #2 -x+1,y,-z+3/2

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C24 H70 N6 O30 S2.

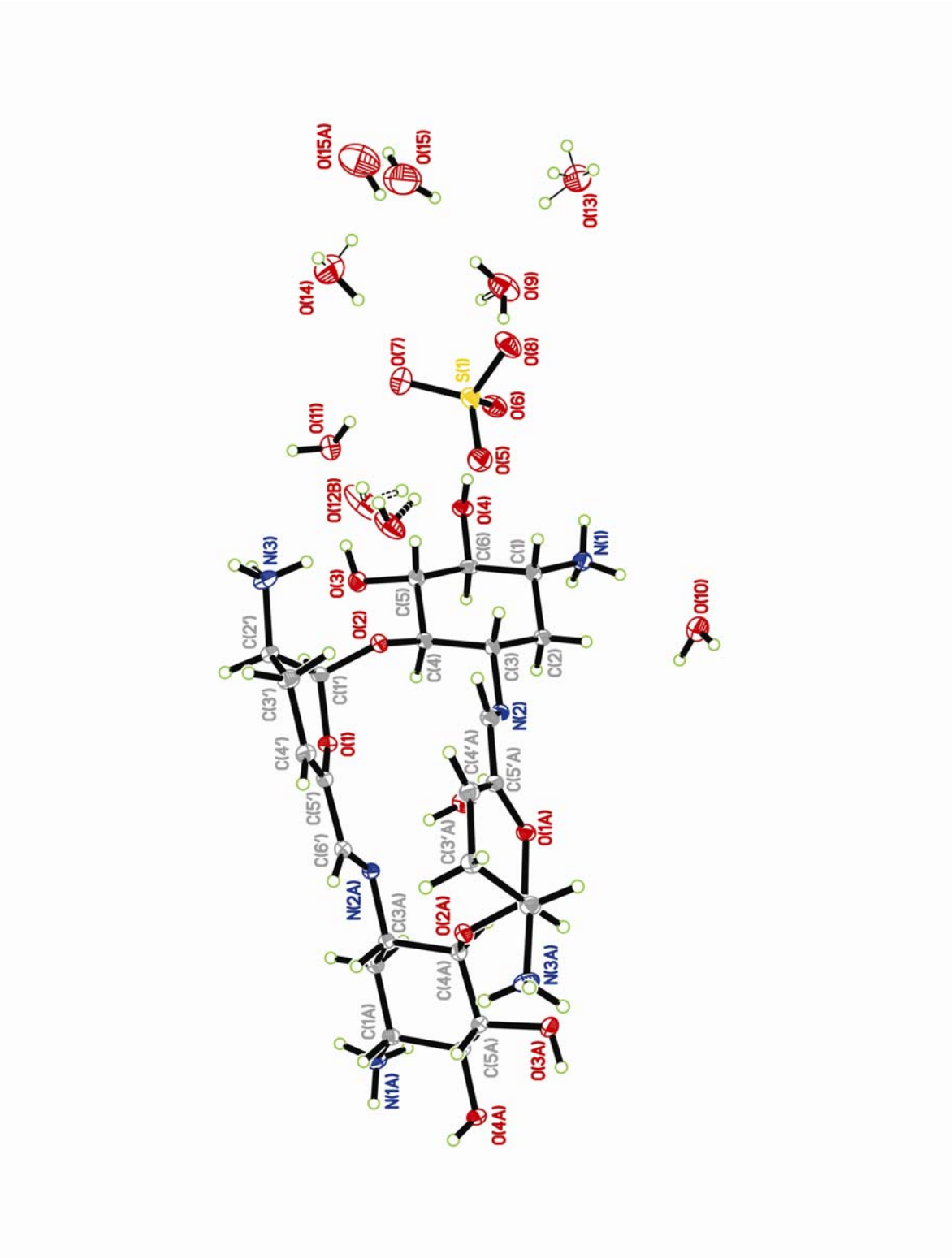
D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(3)-H(3)	O(11)	0.84	2.13	2.925(2)	159.1
O(4)-H(4)	O(6)	0.84	1.91	2.731(2)	165.5
N(1)-H(1C)	O(10)	0.91	2.04	2.914(2)	159.9
N(3)-H(3C)	O(12A)	0.91	1.97	2.857(6)	165.6
N(3)-H(3C)	O(12B)	0.91	1.72	2.582(10)	156.7
O(9)-H(9A)	O(6)	0.871(10)	2.026(17)	2.870(3)	163(4)
O(9)-H(9B)	O(15)	0.873(10)	2.354(17)	3.205(7)	165(5)
O(11)-H(11B)	O(7)	0.867(10)	1.965(14)	2.814(3)	166(4)
O(12A)-H(12A)	O(5)	0.862(10)	1.913(19)	2.761(6)	167(8)
O(12B)-H(12C)	O(5)	0.861(11)	1.98(2)	2.839(11)	173(13)
O(13)-H(13B)	O(9)	0.873(10)	2.02(5)	2.793(3)	147(9)
O(14)-H(14A)	O(7)	0.876(10)	2.087(19)	2.919(3)	158(4)
O(14)-H(14B)	O(15)	0.867(10)	1.765(18)	2.624(8)	171(9)
O(15)-H(15B)	O(9)	0.861(10)	2.42(3)	3.205(7)	151(5)
O(16)-H(16A)	N(2)	0.874(10)	1.988(14)	2.827(2)	160(3)
N(1)-H(1A)	O(4)#3	0.91	1.96	2.818(2)	156.8
N(1)-H(1B)	O(11)#3	0.91	2.07	2.793(2)	135.1
N(3)-H(3A)	O(8)#4	0.91	1.84	2.741(2)	171.6
N(3)-H(3B)	O(5)#5	0.91	2.05	2.843(3)	144.7
N(3)-H(3B)	O(8)#5	0.91	2.52	3.302(3)	144.6
O(9)-H(9C)	O(10)#6	0.866(10)	1.94(2)	2.791(3)	165(8)
O(10)-H(10A)	O(16)#7	0.872(10)	1.928(11)	2.794(2)	173(3)
O(10)-H(10B)	O(13)#6	0.859(10)	2.009(15)	2.817(3)	156(3)
O(11)-H(11A)	O(8)#5	0.875(10)	1.872(12)	2.737(2)	169(3)
O(12A)-H(12B)	O(7)#8	0.856(10)	1.88(3)	2.704(6)	161(8)
O(12B)-H(12D)	O(7)#8	0.858(10)	1.97(4)	2.809(10)	165(13)
O(13)-H(13A)	O(14)#7	0.873(10)	1.92(2)	2.789(4)	170(9)
O(13)-H(13C)	O(13)#9	0.873(10)	1.969(16)	2.791(5)	156(3)
O(14)-H(14B)	O(15)#2	0.867(10)	2.01(3)	2.802(7)	152(5)
O(15)-H(15A)	O(14)#2	0.861(10)	2.31(13)	2.802(7)	117(12)

Symmetry transformations used to generate equivalent atoms:

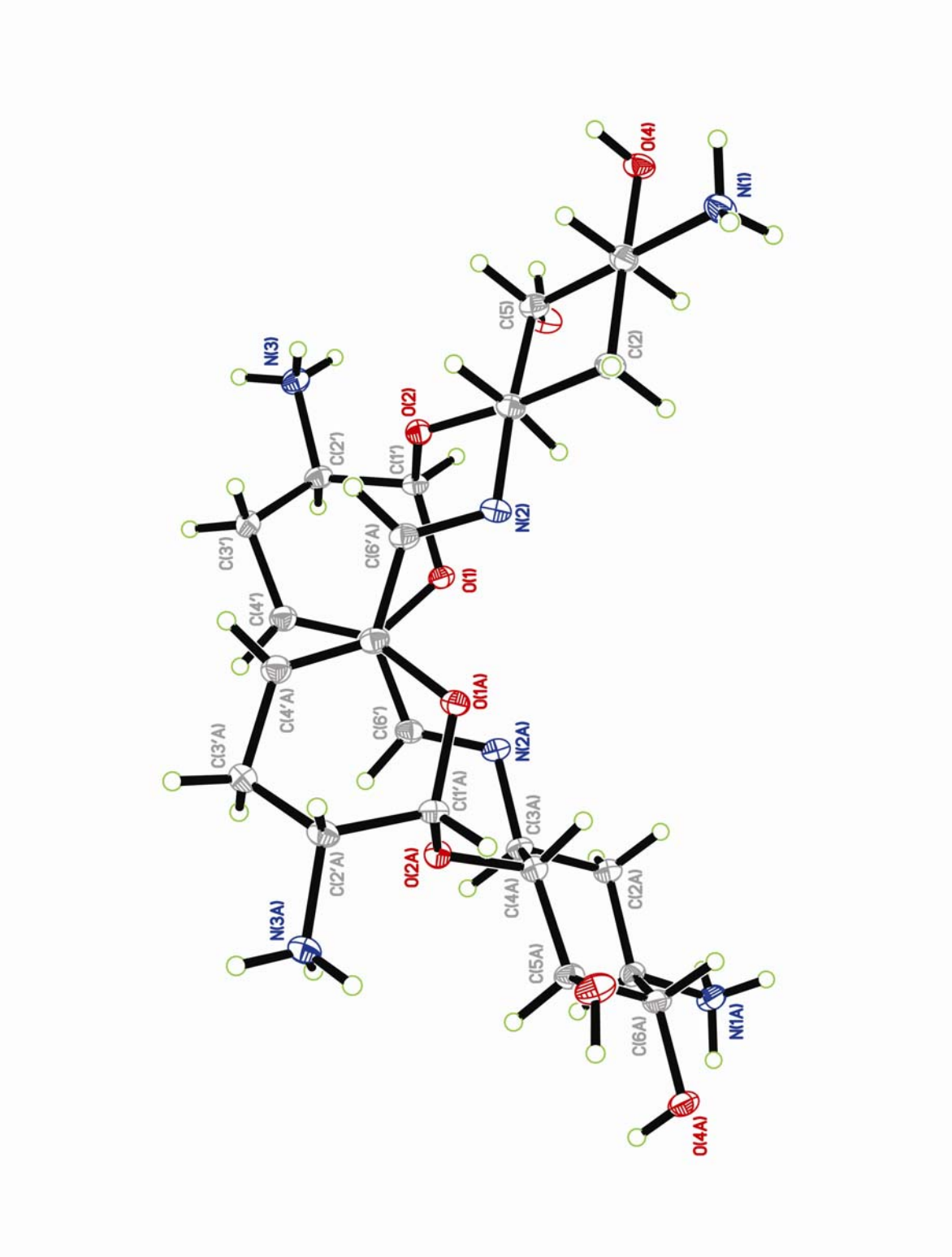
#1 -x,y,-z+1/2 #2 -x+1,y,-z+3/2 #3 x+1/2,-y+1/2,-z+1
#4 x-1,-y,-z+1 #5 x-1,y,z #6 x-1/2,-y+1/2,-z+1
#7 x+1,y,z #8 x,-y,-z+1 #9 -x+2,y,-z+3/2



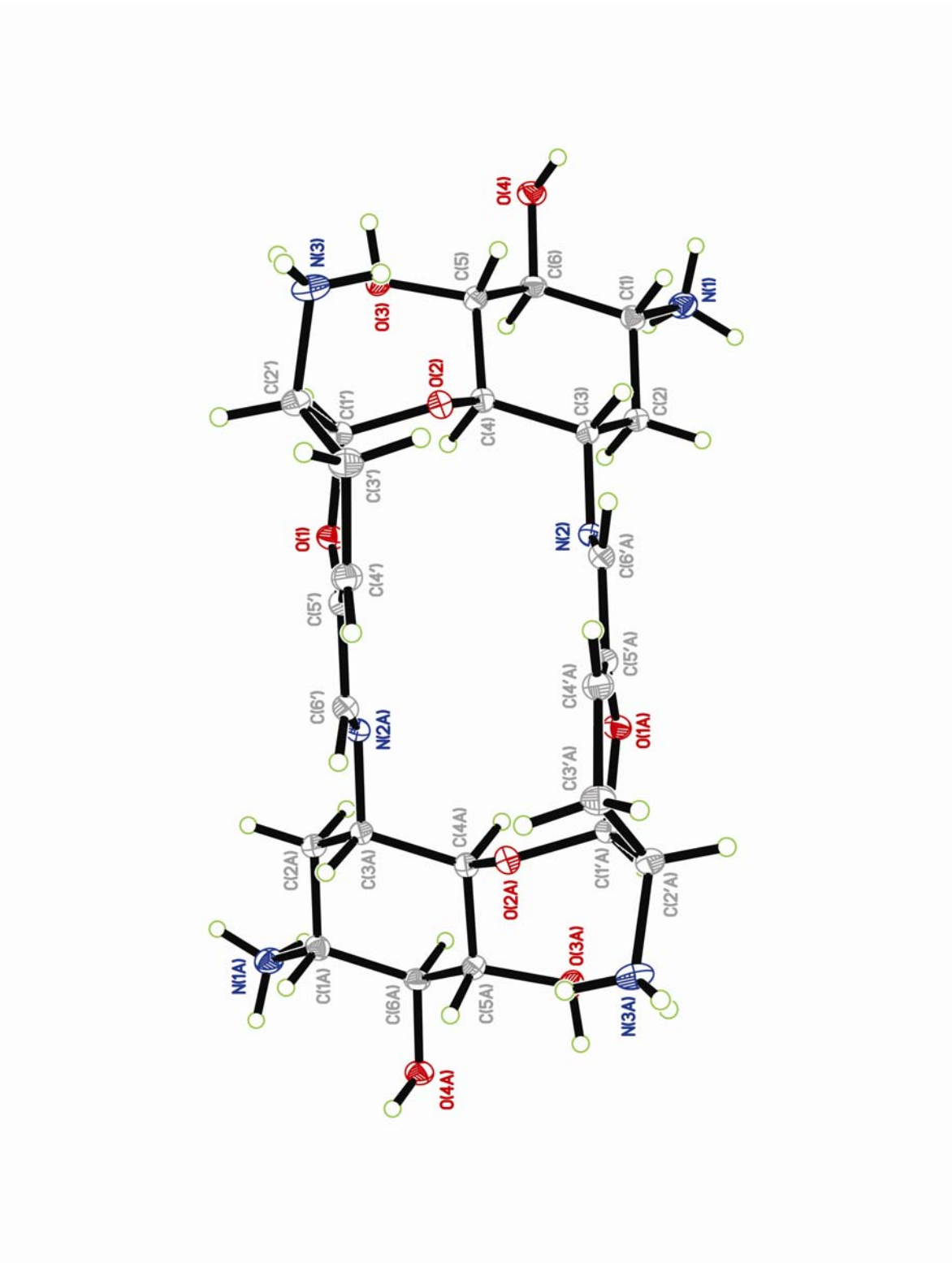
ORTEP (asymmetric unit) view of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



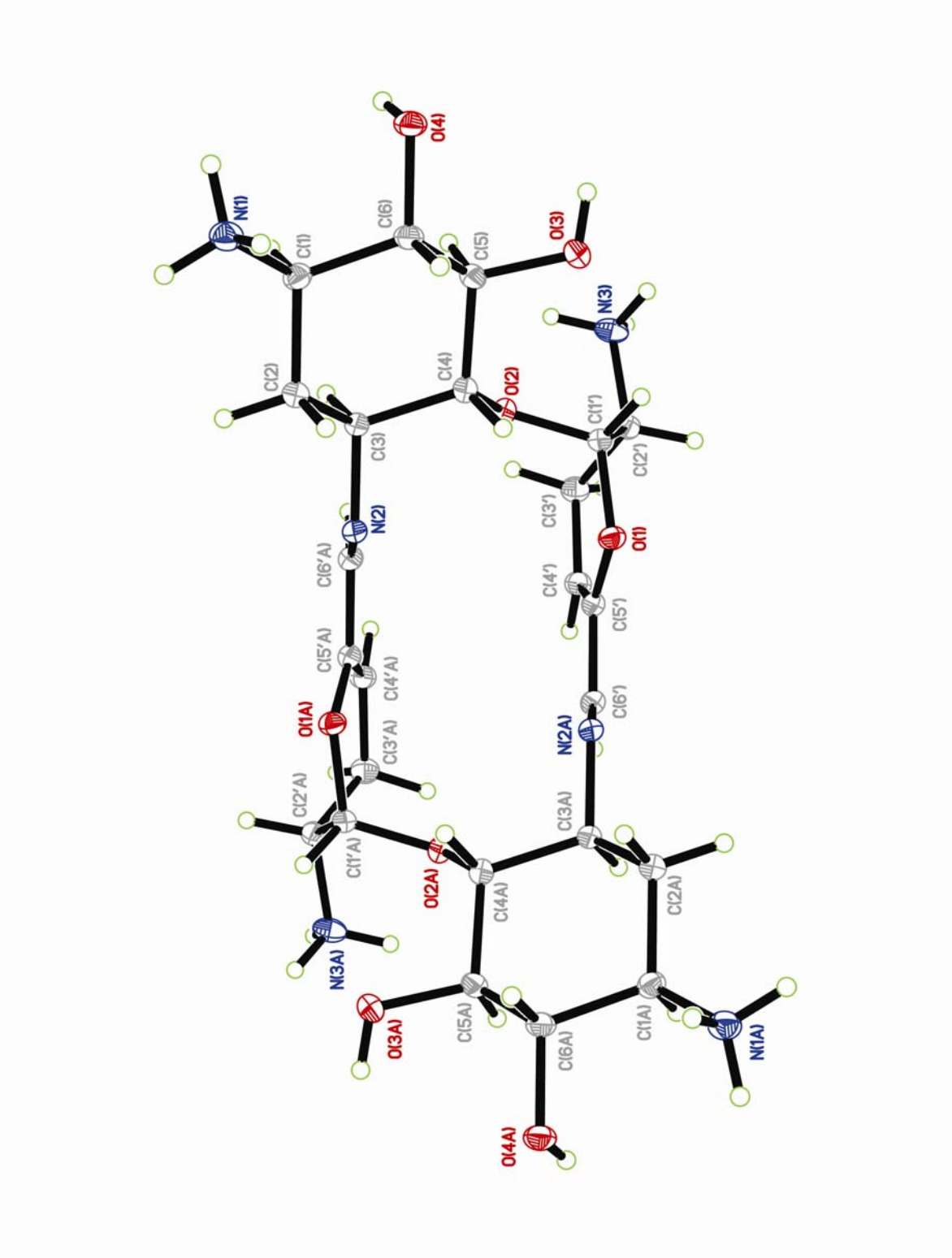
ORTEP view of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP side view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP top view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP bottom view (molecule only) of the C24 H70 N6 O30 S2 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

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Cell: a=6.7453(1) b=25.6806(5) c=25.6822(5)
alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	4448.76(14)	4448.76(14)
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Hall group	C 2c 2	C 2c 2
Moiety formula	C24 H42 N6 O8, 2(O4 S), 14(H2 O)	C24 H42 N6 O8, 2(O4 S), 14(H2 O)
Sum formula	C24 H70 N6 O30 S2	C24 H70 N6 O30 S2
Mr	987.00	986.98
Dx,g cm-3	1.474	1.474
Z	4	4
Mu (mm-1)	2.005	2.005
F000	2112.0	2112.0
F000'	2122.78	
h,k,lmax	8,31,31	8,31,31
Nref	2511[4432]	4389
Tmin,Tmax	0.805,0.961	0.778,0.961
Tmin'	0.486	

Correction method= MULTI-SCAN
Data completeness= 1.75/0.99 Theta(max)= 72.540
R(reflections)= 0.0335(4200) wR2(reflections)= 0.1030(4389)
S = 1.073 Npar= 364

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level B

PLAT420_ALERT_2_B D-H Without Acceptor O14 - *H14C ... ?

Author Response: This is attributed to a disordered hydrogen bond network resulting from a disordered water molecule (O15) which may appear on either side of the corresponding symmetry element.

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.
From the CIF: _diffrn_reflns_theta_max 72.54
From the CIF: _reflns_number_total 4389
Count of symmetry unique reflns 2511
Completeness (_total/calc) 174.79%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 1878
Fraction of Friedel pairs measured 0.748
Are heavy atom types Z>Si present yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 30
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ..... 12 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 2
PLAT791_ALERT_4_G Note: The Model has Chirality at C1 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C1' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C2' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C3 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C4 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C5 (Verify) R

PLAT791_ALERT_4_G Note: The Model has Chirality at C6 (Verify) S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 34

0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
0 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
13 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
10 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

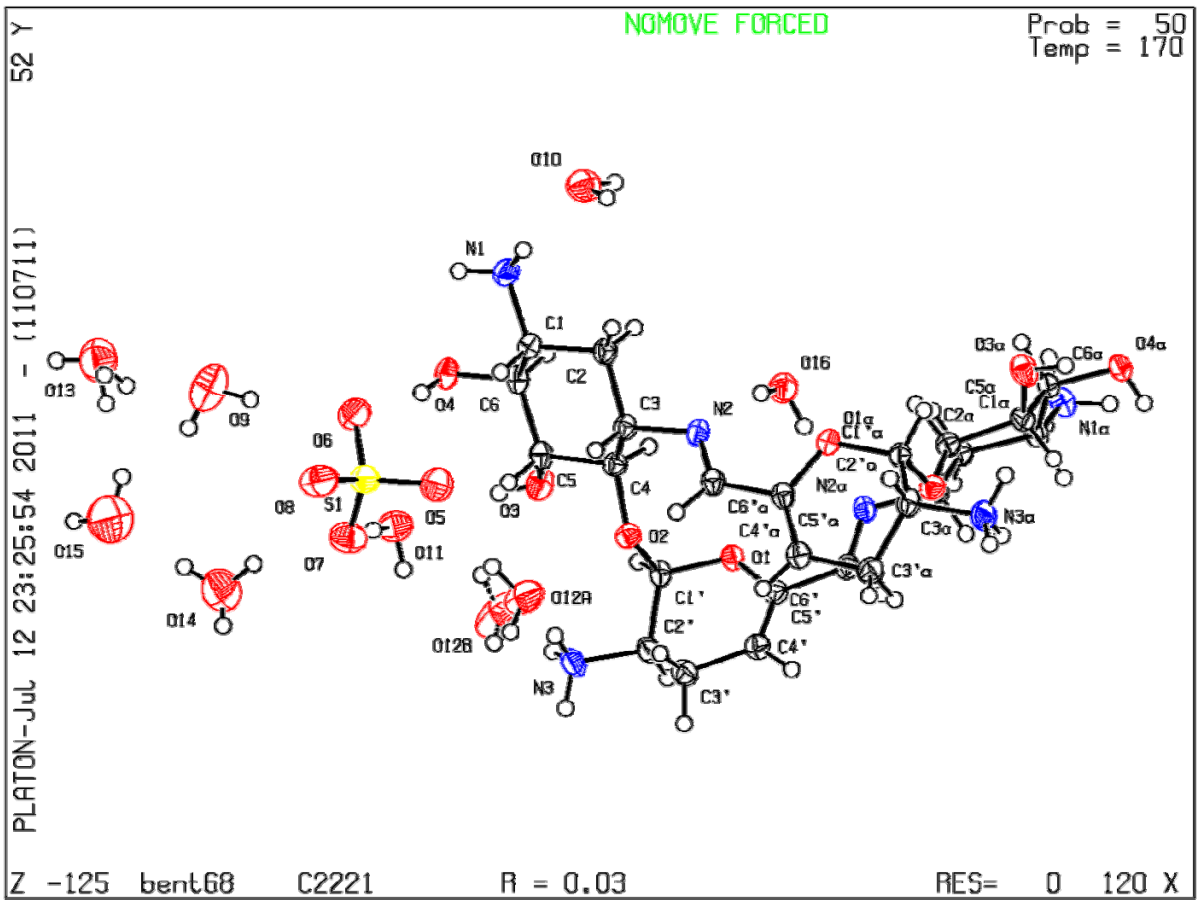
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/07/2011; check.def file version of 04/07/2011

Datablock bent68 - ellipsoid plot



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Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

2(C28 H46 N6 O8) • 5(S O4) • 2(N H4) • 20(H2 O) • 2(C2 H5 O) COMPOUND (bent70)

Equipe Hanessian

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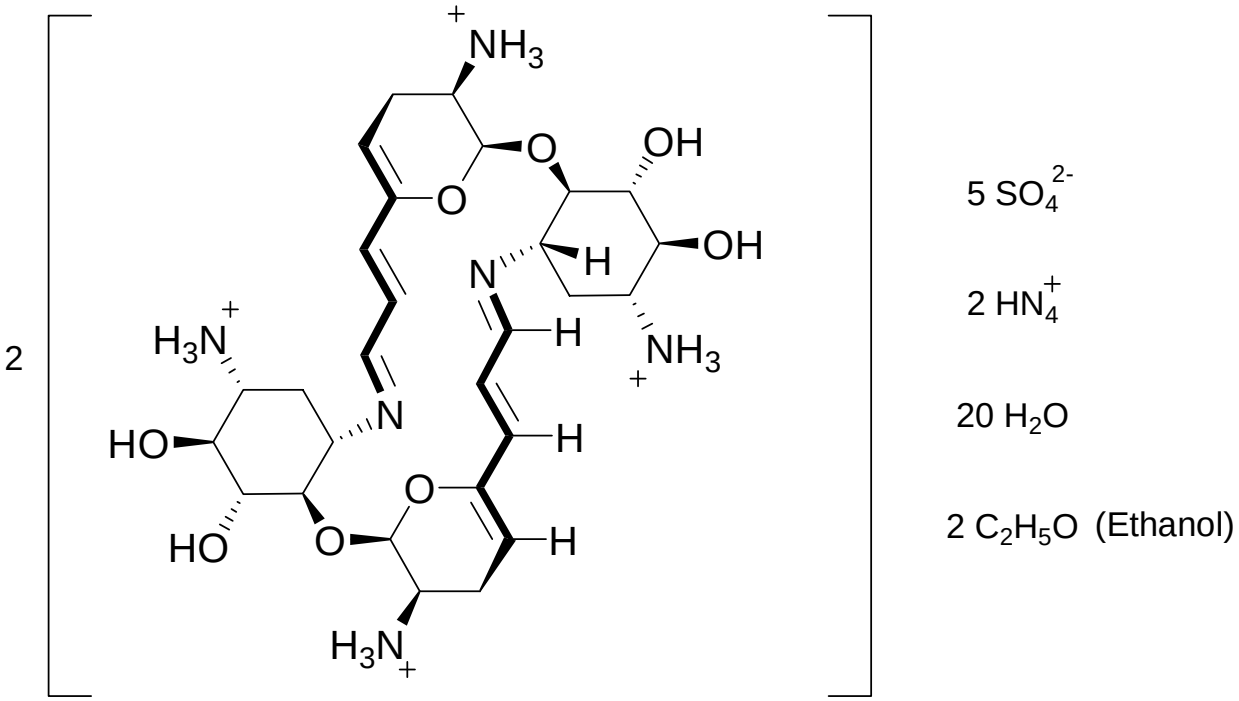


(9 H_2O, 2 C_2H_5O and 1 NH_4^+ Squeezed Out)

Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Benoît Deschênes Simard.

Table 1. Crystal data and structure refinement for C56 H118 N13 O47 S5.

Identification code	bent70
Empirical formula without squeeze	2(C28 H46 N6 O8) • 5(S O4) • 2(N H4) • 20(H2 O) • 2(C2 H5 O)
Empirical formula squeezed (ions and solvent)	2(C28 H46 N6 O8) • 5(S O4) • 1(N H4) • 11(H2 O)
Empirical formula squeezed	C56 H118 N13 O47 S5
Formula weight	942.97
Temperature	150K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 6.6138(4) Å α = 101.113(3)° b = 16.3922(10) Å β = 92.328(3)° c = 23.9598(14) Å γ = 95.176(3)°
Volume	2534.0(3)Å^3
Z	1
Density (calculated)	1.236 g/cm^3 (without squeeze: 1.413 g/cm^3)
Absorption coefficient	1.835 mm^{-1} (without squeeze: 1.988 mm^{-1})
F(000)	1001 (without squeeze: 1152)
Crystal size	0.37 x 0.03 x 0.02 mm
Theta range for data collection	2.76 to 69.17°
Index ranges	$-7 \le h \le 7$, $-19 \le k \le 18$, $-28 \le \ell \le 20$
Reflections collected	42684
Independent reflections	12907 [R_{int} = 0.055]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9640 and 0.5025
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12907 / 343 / 1168
Goodness-of-fit on F^2	0.969

Final R indices [I>2sigma(I)]	R_1 = 0.0766, wR_2 = 0.1888
R indices (all data)	R_1 = 0.0893, wR_2 = 0.1971
Absolute structure parameter	0.10(2)
Largest diff. peak and hole	1.126 and -0.674 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C56 H118 N13 O47 S5.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U_{eq}
S(1)	782(2)	279(1)	12944(1)	30(1)
O(51)	44(6)	-545(3)	13059(2)	43(1)
O(52)	779(8)	939(3)	13450(2)	56(1)
O(53)	2856(5)	229(3)	12743(2)	37(1)
O(54)	-583(6)	472(3)	12494(2)	35(1)
S(2)	7558(2)	561(1)	8274(1)	29(1)
O(61)	6749(6)	-265(2)	8360(2)	35(1)
O(62)	6282(5)	786(3)	7815(2)	33(1)
O(63)	7432(7)	1191(3)	8783(2)	49(1)
O(64)	9678(5)	523(3)	8108(2)	36(1)
S(3)	2521(3)	9118(1)	5263(1)	57(1)
O(71)	4491(9)	9303(4)	5564(3)	75(2)
O(72)	1638(9)	8269(4)	5226(3)	80(2)
O(73)	1172(13)	9721(5)	5508(3)	110(3)
O(74)	2812(11)	9222(4)	4690(3)	89(2)
S(4)	5898(2)	8717(1)	10015(1)	37(1)
O(81)	6050(7)	7976(3)	10275(2)	51(1)
O(82)	8012(6)	9130(3)	10031(2)	42(1)
O(83)	4671(8)	9315(4)	10347(3)	73(2)
O(84)	5094(6)	8461(3)	9435(2)	45(1)
S(5)	6979(3)	1456(2)	14769(1)	70(1)
O(91)	6168(8)	1042(3)	14195(2)	55(1)
O(92)	8397(11)	2219(5)	14762(5)	129(3)
O(93)	5392(11)	1768(5)	15113(3)	90(2)
O(94)	7923(10)	836(5)	15022(3)	91(2)
O(11)	993(5)	2521(2)	7788(2)	28(1)
O(12)	3631(6)	3606(3)	7918(2)	36(1)
O(13)	2118(5)	1177(3)	6894(2)	36(1)
O(14)	-1418(6)	192(3)	6305(2)	37(1)
N(11)	-4801(8)	1015(4)	6056(2)	44(1)
N(12)	-1623(7)	3587(3)	7272(3)	42(1)
N(13)	3244(7)	1595(3)	8430(2)	30(1)
C(11)	5568(8)	8500(4)	6994(3)	30(1)
C(12)	5230(9)	7583(4)	6989(3)	36(2)
C(13)	4205(8)	7411(4)	7529(3)	30(1)
C(14)	2194(8)	7801(4)	7592(3)	29(1)
C(15)	2379(8)	8725(4)	7530(3)	34(2)
C(16)	3504(8)	8893(4)	7014(3)	31(1)
C(11')	-514(8)	7559(4)	8211(3)	31(1)
C(12')	-972(8)	7961(4)	8813(2)	30(1)
C(13')	268(9)	7597(4)	9235(3)	32(1)
C(14')	5(9)	6690(5)	9073(3)	42(2)
C(15')	-663(8)	6279(4)	8550(3)	37(2)
C(16')	-1011(8)	5409(4)	8394(3)	42(2)
C(17')	-1326(8)	4928(4)	7867(3)	41(2)
C(18')	-1589(8)	4036(4)	7764(3)	39(2)
O(21)	1569(5)	7751(3)	8147(2)	32(1)
O(22)	-1073(6)	6685(3)	8107(2)	36(1)
O(23)	358(5)	8950(3)	7512(2)	38(1)

O(24)	3799(6)	9748(3)	7015(2)	37(1)
N(21)	6608(8)	8644(4)	6486(3)	44(1)
N(22)	3886(7)	6502(3)	7484(3)	37(1)
N(23)	-585(7)	8879(3)	8919(2)	30(1)
C(21)	-3345(8)	1382(4)	6539(3)	32(1)
C(22)	-3200(8)	2303(4)	6659(3)	30(1)
C(23)	-1869(8)	2685(4)	7212(3)	34(2)
C(24)	210(8)	2347(4)	7197(3)	32(1)
C(25)	92(8)	1402(4)	6990(3)	31(1)
C(26)	-1237(8)	1081(3)	6439(3)	31(1)
C(21')	3090(7)	2748(4)	7904(3)	29(1)
C(22')	3699(9)	2495(4)	8462(3)	32(1)
C(23')	2564(11)	2995(4)	8938(3)	43(2)
C(24')	2843(10)	3887(5)	8896(3)	44(2)
C(25')	3349(8)	4159(4)	8437(3)	34(2)
C(26')	3719(8)	5011(4)	8391(3)	44(2)
C(27')	3787(8)	5321(4)	7909(3)	36(2)
C(28')	4051(8)	6200(5)	7927(3)	43(2)
O(31)	4080(5)	2182(3)	12408(2)	31(1)
O(32)	6701(6)	3259(3)	12506(2)	35(1)
O(33)	5190(5)	864(2)	11505(2)	30(1)
O(34)	1591(5)	-118(2)	10918(2)	32(1)
N(31)	-1729(6)	749(3)	10652(2)	30(1)
N(32)	1519(7)	3263(3)	11912(2)	35(1)
N(33)	6356(7)	1298(3)	13074(2)	31(1)
C(31)	-272(7)	1071(4)	11161(2)	28(1)
C(32)	-95(8)	2020(4)	11290(3)	28(1)
C(33)	1204(7)	2347(4)	11837(3)	27(1)
C(34)	3308(7)	2005(4)	11828(2)	25(1)
C(35)	3130(7)	1077(3)	11598(2)	23(1)
C(36)	1820(7)	776(3)	11058(2)	26(1)
C(31')	6194(8)	2409(4)	12515(3)	30(1)
C(32')	6799(9)	2209(4)	13085(3)	33(1)
C(33')	5623(10)	2728(4)	13546(3)	43(2)
C(34')	5917(10)	3612(4)	13491(3)	45(2)
C(35')	6428(9)	3825(4)	12994(3)	39(2)
C(36')	6745(8)	4684(4)	12949(3)	43(2)
C(37')	6814(8)	4973(5)	12456(3)	45(2)
C(38')	7099(8)	5862(4)	12463(3)	38(2)
O(41)	4722(5)	7387(3)	12768(2)	30(1)
O(42)	2007(5)	6363(3)	12744(2)	36(1)
O(43)	3493(5)	8666(3)	12217(2)	39(1)
O(44)	6844(6)	9499(3)	11707(2)	36(1)
N(41)	9441(7)	8390(3)	11075(2)	38(1)
N(42)	6888(7)	6177(3)	12033(2)	37(1)
N(43)	2793(8)	8566(3)	13534(2)	35(1)
C(41)	8523(8)	8224(4)	11606(3)	31(1)
C(42)	8167(8)	7297(4)	11578(3)	33(1)
C(43)	7249(8)	7089(4)	12101(3)	31(1)
C(44)	5290(8)	7477(4)	12214(3)	31(1)
C(45)	5519(7)	8411(4)	12196(3)	33(1)
C(46)	6519(8)	8616(4)	11674(3)	29(1)
C(41')	2599(8)	7246(4)	12840(3)	33(1)
C(42')	2231(8)	7665(4)	13444(3)	33(1)
C(43')	3422(11)	7284(4)	13871(3)	43(2)
C(44')	3041(11)	6354(5)	13721(3)	45(2)
C(45')	2368(9)	5962(4)	13198(3)	37(2)
C(46')	2007(8)	5068(4)	13042(3)	40(2)
C(47')	1762(8)	4609(4)	12510(3)	38(2)
C(48')	1494(8)	3717(4)	12414(3)	38(2)
O(101)	3401(7)	1315(3)	9576(2)	47(1)
O(102)	3488(6)	9692(3)	9052(2)	42(1)

O(103)	2516(7)	7397(3)	10766(2)	57(1)
O(104)	2864(7)	3717(3)	10897(2)	72(2)
O(105)	9444(7)	1599(3)	9788(2)	53(1)
O(106)	9191(9)	3299(4)	10184(3)	75(2)
O(107)	2223(9)	5715(4)	10280(3)	80(2)
O(108)	5259(9)	5192(4)	10962(3)	76(2)
O(109)	5392(11)	6276(5)	9655(4)	107(3)
O(110)	8172(11)	5048(5)	10042(4)	120(3)
O(111)	5475(8)	2479(4)	10492(3)	69(2)
N(101)	1814(10)	856(5)	14550(3)	72(2)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C56 H118 N13 O47 S5.

	x	y	z	U_{eq}
H(13)	2712	1150	7205	55
H(14)	-1502	29	5949	56
H(11A)	-4765	451	5974	65
H(11B)	-4462	1233	5747	65
H(11C)	-6076	1135	6149	65
H(13A)	3508	1473	8779	44
H(13B)	4033	1311	8173	44
H(13C)	1909	1443	8319	44
H(11)	6446	8775	7341	36
H(12A)	6553	7343	6966	43
H(12B)	4361	7305	6647	43
H(13D)	5136	7657	7870	36
H(14A)	1155	7471	7301	34
H(15)	3124	9069	7881	41
H(16)	2647	8618	6663	38
H(11')	-1318	7808	7935	37
H(12')	-2445	7814	8863	35
H(13E)	1723	7801	9234	39
H(13F)	-191	7777	9624	39
H(14')	322	6373	9353	50
H(16')	-1028	5117	8699	50
H(17')	-1375	5196	7549	49
H(18')	-1746	3768	8080	47
H(23)	380	9472	7570	57
H(24)	3908	10017	7353	55
H(21A)	7811	8413	6476	66
H(21B)	6847	9203	6500	66
H(21C)	5811	8404	6168	66
H(23A)	-489	9084	9301	44
H(23B)	-1625	9094	8755	44
H(23C)	600	9025	8767	44
H(21)	-3849	1188	6884	39
H(22A)	-4582	2487	6699	36
H(22B)	-2608	2513	6335	36
H(23D)	-2577	2539	7546	41
H(24A)	1129	2640	6961	38
H(25)	-463	1123	7295	37
H(26)	-629	1311	6120	38
H(21')	3824	2419	7594	34
H(22')	5195	2645	8546	38
H(23E)	1099	2793	8897	52
H(23F)	3111	2924	9315	52
H(24')	2641	4291	9226	53
H(26')	3944	5407	8739	53
H(27')	3656	4947	7550	43
H(28')	4361	6568	8284	51
H(33)	5317	394	11586	46
H(34)	2429	-284	10678	48
H(31A)	-1325	985	10356	45
H(31B)	-2999	884	10740	45
H(31C)	-1746	184	10553	45
H(33A)	5059	1127	12930	46

H(33B)	6499	1201	13434	46
H(33C)	7238	1010	12850	46
H(31)	-814	862	11497	34
H(32A)	531	2236	10972	34
H(32B)	-1464	2216	11330	34
H(33D)	467	2195	12164	33
H(34A)	4228	2302	11594	30
H(35)	2578	785	11898	28
H(36)	2427	1008	10739	31
H(31')	6928	2064	12213	35
H(32')	8291	2370	13170	39
H(33E)	4158	2526	13497	51
H(33F)	6133	2671	13929	51
H(34')	5745	4039	13810	54
H(36')	6923	5087	13294	51
H(37')	6675	4589	12102	54
H(38')	7470	6228	12818	46
H(43G)	3536	9163	12393	58
H(44B)	7615	9716	11994	53
H(41A)	10507	8079	11001	57
H(41B)	9885	8942	11122	57
H(41C)	8489	8249	10778	57
H(43A)	4080	8664	13426	52
H(43B)	2734	8796	13910	52
H(43C)	1915	8799	13324	52
H(41)	9479	8479	11940	37
H(42A)	7252	7042	11241	39
H(42B)	9479	7052	11531	39
H(43D)	8237	7306	12435	37
H(44A)	4204	7182	11924	38
H(45)	6342	8719	12545	39
H(46)	5592	8370	11331	35
H(41')	1817	7501	12563	39
H(42')	749	7567	13505	39
H(43E)	4894	7455	13864	51
H(43F)	2993	7486	14261	51
H(44')	3284	6035	14004	54
H(46')	1935	4771	13345	48
H(47')	1766	4882	12194	45
H(48')	1291	3452	12730	46
H(1E)	3940(80)	851(19)	9550(20)	70
H(1F)	3540(80)	1540(30)	9936(7)	70
H(2A)	3750(70)	9360(20)	9280(17)	63
H(2B)	4620(40)	9800(20)	8900(17)	63
H(3A)	2460(100)	6860(10)	10740(40)	85
H(3B)	3630(50)	7510(40)	10610(30)	85
H(4A)	1755	3584	10689	107
H(4B)	3643	3336	10780	107
H(5A)	8240(30)	1520(40)	9600(17)	79
H(5B)	10090(80)	1240(40)	9540(30)	79
H(6A)	8870(40)	3015(14)	9837(9)	113
H(6B)	8901	3796	10155	113
H(7A)	3152	5560	10500	120
H(7B)	1680(50)	5228(16)	10086(17)	120
H(8A)	6520(30)	5140(40)	11070(20)	115
H(8B)	4700(100)	4674(19)	10900(50)	115
H(9A)	5450(140)	6821(14)	9700(60)	160
H(9B)	4260(40)	6150(50)	9800(30)	160
H(10A)	7383	5413	9953	180
H(10B)	8600(60)	5270(30)	10391(9)	180
H(11D)	6190(40)	2066(15)	10510(20)	104
H(11E)	6250(70)	2825(17)	10350(30)	104

H(1A)	2520(60)	1240(20)	14385(17)	109
H(1B)	2650(50)	530(20)	14670(20)	109
H(1C)	1170(70)	1130(30)	14841(16)	109
H(1D)	890(60)	550(30)	14290(17)	109

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C56 H118 N13 O47 S5.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
S(1)	26(1)	30(1)	35(1)	5(1)	4(1)	6(1)
O(51)	39(2)	39(3)	59(3)	23(2)	16(2)	14(2)
O(52)	61(3)	62(4)	41(3)	-12(2)	2(2)	26(2)
O(53)	19(2)	38(3)	56(3)	9(2)	13(2)	8(2)
O(54)	28(2)	41(3)	35(2)	8(2)	-7(2)	3(2)
S(2)	23(1)	29(1)	34(1)	3(1)	0(1)	4(1)
O(61)	27(2)	25(2)	55(3)	13(2)	5(2)	4(2)
O(62)	24(2)	48(3)	27(2)	11(2)	-3(2)	7(2)
O(63)	52(3)	52(3)	41(3)	-1(2)	-6(2)	16(2)
O(64)	17(2)	32(3)	59(3)	9(2)	9(2)	5(2)
S(3)	61(1)	57(1)	48(1)	-7(1)	9(1)	6(1)
O(71)	78(4)	66(4)	70(4)	-9(3)	-32(3)	1(3)
O(72)	59(3)	67(4)	103(5)	-2(4)	-9(3)	-5(3)
O(73)	135(6)	99(6)	108(5)	9(4)	65(5)	72(5)
O(74)	120(5)	96(5)	49(4)	-9(3)	-1(3)	55(4)
S(4)	30(1)	37(1)	42(1)	1(1)	6(1)	2(1)
O(81)	45(2)	50(3)	57(3)	13(3)	-3(2)	-10(2)
O(82)	28(2)	42(3)	48(3)	-5(2)	3(2)	-9(2)
O(83)	41(3)	70(4)	94(4)	-23(3)	18(3)	10(2)
O(84)	32(2)	50(3)	48(3)	0(2)	-8(2)	-2(2)
S(5)	66(1)	74(2)	71(1)	18(1)	-4(1)	8(1)
O(91)	59(3)	75(4)	34(3)	14(3)	4(2)	15(3)
O(92)	73(5)	102(6)	220(11)	62(7)	-2(5)	-16(4)
O(93)	104(5)	107(6)	62(4)	6(4)	10(4)	44(4)
O(94)	77(4)	115(6)	93(5)	45(4)	-5(4)	24(4)
O(11)	17(2)	30(2)	35(2)	1(2)	-6(2)	-1(2)
O(12)	29(2)	32(3)	46(3)	8(2)	-1(2)	-1(2)
O(13)	14(2)	35(3)	59(3)	8(2)	-4(2)	5(2)
O(14)	30(2)	32(3)	43(3)	-7(2)	3(2)	-3(2)
N(11)	33(3)	45(4)	45(3)	-6(3)	-4(2)	-2(2)
N(12)	28(2)	34(3)	59(4)	-3(3)	2(2)	6(2)
N(13)	25(2)	31(3)	32(3)	4(2)	-2(2)	6(2)
C(11)	28(3)	29(3)	32(3)	4(3)	1(2)	1(2)
C(12)	30(3)	30(4)	50(4)	6(3)	6(3)	11(2)
C(13)	25(3)	28(4)	34(3)	2(3)	3(2)	2(2)
C(14)	23(2)	23(3)	39(3)	0(3)	2(2)	5(2)
C(15)	20(2)	38(4)	46(4)	7(3)	3(2)	13(2)
C(16)	30(3)	26(3)	36(3)	4(3)	-5(2)	0(2)
C(11')	23(3)	30(4)	37(3)	4(3)	4(2)	0(2)
C(12')	20(2)	37(4)	31(3)	5(3)	1(2)	5(2)
C(13')	34(3)	35(4)	25(3)	1(3)	1(2)	6(2)
C(14')	35(3)	48(5)	44(4)	13(3)	5(3)	4(3)
C(15')	27(3)	32(4)	54(4)	11(3)	3(3)	-1(2)
C(16')	25(3)	34(4)	63(5)	7(4)	3(3)	-6(2)
C(17')	23(3)	36(4)	59(4)	-2(3)	7(3)	8(2)
C(18')	25(3)	37(4)	52(4)	2(3)	2(3)	5(2)
O(21)	16(2)	43(3)	36(2)	6(2)	1(2)	-1(2)
O(22)	33(2)	29(3)	42(3)	2(2)	1(2)	-2(2)
O(23)	20(2)	26(2)	66(3)	2(2)	1(2)	7(2)

O(24)	39(2)	24(2)	43(3)	3(2)	-8(2)	0(2)
N(21)	42(3)	36(3)	53(4)	9(3)	5(3)	-4(2)
N(22)	31(2)	26(3)	57(4)	9(3)	15(2)	7(2)
N(23)	31(2)	23(3)	32(3)	0(2)	0(2)	1(2)
C(21)	23(3)	29(4)	40(3)	-2(3)	-1(2)	-1(2)
C(22)	30(3)	29(4)	29(3)	1(3)	-2(2)	3(2)
C(23)	19(2)	39(4)	44(4)	8(3)	-2(2)	5(2)
C(24)	28(3)	34(4)	32(3)	5(3)	4(2)	4(2)
C(25)	22(3)	31(4)	39(3)	5(3)	2(2)	9(2)
C(26)	27(3)	22(3)	42(4)	-1(3)	-2(2)	2(2)
C(21')	20(2)	24(3)	40(3)	2(3)	0(2)	1(2)
C(22')	32(3)	24(3)	36(3)	1(3)	-3(2)	0(2)
C(23')	58(4)	33(4)	37(4)	6(3)	-1(3)	5(3)
C(24')	43(3)	44(4)	41(4)	-3(3)	2(3)	8(3)
C(25')	29(3)	24(4)	48(4)	4(3)	-5(3)	-3(2)
C(26')	29(3)	37(4)	62(5)	-4(4)	-1(3)	3(3)
C(27')	25(3)	27(4)	58(4)	11(3)	3(3)	7(2)
C(28')	21(3)	49(5)	57(5)	9(4)	8(3)	0(3)
O(31)	20(2)	36(3)	34(2)	4(2)	-3(2)	-2(2)
O(32)	27(2)	35(3)	42(3)	10(2)	-7(2)	-5(2)
O(33)	15(2)	21(2)	56(3)	6(2)	7(2)	5(1)
O(34)	24(2)	21(2)	46(3)	-6(2)	7(2)	-2(2)
N(31)	19(2)	27(3)	39(3)	-7(2)	-5(2)	-3(2)
N(32)	25(2)	30(3)	49(3)	3(3)	-3(2)	10(2)
N(33)	28(2)	23(3)	41(3)	10(2)	-5(2)	2(2)
C(31)	15(2)	37(4)	31(3)	2(3)	-4(2)	-1(2)
C(32)	26(3)	25(3)	31(3)	-2(3)	0(2)	4(2)
C(33)	17(2)	28(3)	34(3)	-1(3)	-1(2)	8(2)
C(34)	18(2)	27(3)	31(3)	6(3)	5(2)	8(2)
C(35)	17(2)	22(3)	31(3)	2(2)	3(2)	7(2)
C(36)	21(2)	24(3)	30(3)	0(3)	0(2)	2(2)
C(31')	28(3)	27(4)	33(3)	5(3)	1(2)	-1(2)
C(32')	32(3)	33(4)	32(3)	1(3)	0(2)	6(2)
C(33')	47(3)	45(4)	37(4)	8(3)	6(3)	6(3)
C(34')	54(4)	34(4)	46(4)	2(3)	-2(3)	9(3)
C(35')	36(3)	30(4)	48(4)	6(3)	-7(3)	0(3)
C(36')	34(3)	38(4)	54(4)	10(4)	-10(3)	-2(3)
C(37')	17(3)	52(5)	65(5)	9(4)	1(3)	5(2)
C(38')	21(3)	30(4)	65(5)	13(3)	-3(3)	3(2)
O(41)	21(2)	37(3)	28(2)	3(2)	-2(2)	-1(2)
O(42)	26(2)	34(3)	41(3)	-1(2)	-2(2)	-11(2)
O(43)	25(2)	27(2)	60(3)	-2(2)	3(2)	8(2)
O(44)	34(2)	30(3)	42(2)	4(2)	-4(2)	7(2)
N(41)	37(3)	27(3)	46(3)	-1(3)	13(2)	1(2)
N(42)	30(2)	30(3)	51(3)	9(3)	8(2)	10(2)
N(43)	40(3)	32(3)	28(3)	-3(2)	3(2)	5(2)
C(41)	24(3)	25(3)	44(4)	2(3)	0(2)	9(2)
C(42)	19(2)	32(4)	47(4)	5(3)	4(2)	5(2)
C(43)	23(3)	21(3)	44(4)	-2(3)	1(2)	1(2)
C(44)	20(2)	37(4)	37(3)	5(3)	3(2)	7(2)
C(45)	22(2)	28(4)	45(4)	2(3)	2(2)	1(2)
C(46)	24(2)	22(3)	41(3)	3(3)	-1(2)	6(2)
C(41')	19(2)	32(4)	44(4)	1(3)	-2(2)	-3(2)
C(42')	28(3)	35(4)	32(3)	3(3)	-2(2)	-5(2)
C(43')	56(4)	43(4)	32(4)	11(3)	3(3)	8(3)
C(44')	58(4)	43(4)	37(4)	12(3)	6(3)	11(3)
C(45')	38(3)	28(4)	43(4)	7(3)	5(3)	-1(2)
C(46')	39(3)	33(4)	45(4)	2(3)	12(3)	0(3)
C(47')	20(3)	38(4)	48(4)	-6(3)	-2(2)	3(2)
C(48')	24(3)	34(4)	53(4)	0(3)	-1(3)	5(2)
O(101)	50(3)	48(3)	42(3)	9(2)	10(2)	6(2)
O(102)	30(2)	47(3)	51(3)	16(2)	1(2)	4(2)

O(103)	49(3)	50(3)	72(4)	12(3)	24(3)	-1(2)
O(104)	65(3)	66(4)	77(4)	3(3)	7(3)	-8(3)
O(105)	49(3)	64(4)	43(3)	8(3)	-6(2)	2(2)
O(106)	69(4)	67(4)	87(4)	11(3)	-1(3)	3(3)
O(107)	68(4)	53(4)	113(5)	5(4)	-4(3)	-4(3)
O(108)	62(3)	62(4)	103(5)	15(4)	7(3)	-7(3)
O(109)	74(4)	121(6)	103(6)	-18(5)	23(4)	-27(4)
O(110)	74(5)	133(7)	151(8)	40(6)	4(5)	-18(4)
O(111)	57(3)	83(5)	66(4)	13(3)	-2(3)	6(3)
N(101)	46(4)	100(6)	63(4)	-10(4)	-2(3)	18(4)

Table 5. Bond lengths [Å] and angles [°] for C56 H118 N13 O47 S5.

S(1)-O(52)	1.460(5)	C(24)-C(25)	1.527(8)
S(1)-O(51)	1.474(5)	C(25)-C(26)	1.531(8)
S(1)-O(53)	1.477(4)	C(21')-C(22')	1.523(9)
S(1)-O(54)	1.477(4)	C(22')-C(23')	1.537(9)
S(2)-O(63)	1.448(5)	C(23')-C(24')	1.481(10)
S(2)-O(61)	1.465(4)	C(24')-C(25')	1.309(10)
S(2)-O(64)	1.476(4)	C(25')-C(26')	1.422(9)
S(2)-O(62)	1.481(4)	C(26')-C(27')	1.349(10)
S(3)-O(74)	1.434(7)	C(27')-C(28')	1.427(9)
S(3)-O(71)	1.441(6)	O(31)-C(31')	1.414(6)
S(3)-O(72)	1.444(6)	O(31)-C(34)	1.426(7)
S(3)-O(73)	1.447(6)	O(32)-C(35')	1.374(8)
S(4)-O(84)	1.439(5)	O(32)-C(31')	1.409(7)
S(4)-O(83)	1.465(5)	O(33)-C(35)	1.452(5)
S(4)-O(81)	1.477(5)	O(34)-C(36)	1.432(6)
S(4)-O(82)	1.493(4)	N(31)-C(31)	1.503(7)
S(5)-O(93)	1.431(7)	N(32)-C(48')	1.289(8)
S(5)-O(94)	1.454(7)	N(32)-C(33)	1.471(8)
S(5)-O(91)	1.468(6)	N(33)-C(32')	1.490(8)
S(5)-O(92)	1.497(8)	C(31)-C(32)	1.520(8)
O(11)-C(21')	1.405(6)	C(31)-C(36)	1.521(7)
O(11)-C(24)	1.455(7)	C(32)-C(33)	1.516(8)
O(12)-C(21')	1.413(7)	C(33)-C(34)	1.546(6)
O(12)-C(25')	1.419(8)	C(34)-C(35)	1.508(8)
O(13)-C(25)	1.437(6)	C(35)-C(36)	1.502(8)
O(14)-C(26)	1.424(6)	C(31')-C(32')	1.510(9)
N(11)-C(21)	1.471(8)	C(32')-C(33')	1.542(9)
N(12)-C(18')	1.262(9)	C(33')-C(34')	1.477(10)
N(12)-C(23)	1.453(8)	C(34')-C(35')	1.351(10)
N(13)-C(22')	1.465(8)	C(35')-C(36')	1.430(9)
C(11)-N(21)	1.469(8)	C(36')-C(37')	1.356(10)
C(11)-C(12)	1.496(8)	C(37')-C(38')	1.449(9)
C(11)-C(16)	1.560(8)	C(38')-N(42)	1.247(9)
C(12)-C(13)	1.546(9)	O(41)-C(44)	1.425(7)
C(13)-N(22)	1.468(8)	O(41)-C(41')	1.425(6)
C(13)-C(14)	1.528(7)	O(42)-C(45')	1.398(8)
C(14)-O(21)	1.424(7)	O(42)-C(41')	1.437(7)
C(14)-C(15)	1.545(8)	O(43)-C(45)	1.439(5)
C(15)-O(23)	1.419(6)	O(44)-C(46)	1.430(7)
C(15)-C(16)	1.525(9)	N(41)-C(41)	1.492(8)
C(16)-O(24)	1.397(7)	N(42)-C(43)	1.469(8)
C(11')-O(21)	1.407(6)	N(43)-C(42')	1.462(8)
C(11')-O(22)	1.419(7)	C(41)-C(42)	1.505(8)
C(11')-C(12')	1.520(8)	C(41)-C(46)	1.526(7)
C(12')-N(23)	1.474(8)	C(42)-C(43)	1.496(9)
C(12')-C(13')	1.518(8)	C(43)-C(44)	1.506(7)
C(13')-C(14')	1.456(9)	C(44)-C(45)	1.533(9)
C(14')-C(15')	1.340(10)	C(45)-C(46)	1.519(9)
C(15')-O(22)	1.387(8)	C(41')-C(42')	1.518(9)
C(15')-C(16')	1.398(9)	C(42')-C(43')	1.526(9)
C(16')-C(17')	1.351(10)	C(43')-C(44')	1.492(10)
C(17')-C(18')	1.429(9)	C(44')-C(45')	1.333(10)
N(22)-C(28')	1.261(9)	C(45')-C(46')	1.435(9)
C(21)-C(22)	1.475(8)	C(46')-C(47')	1.346(9)
C(21)-C(26)	1.533(7)	C(47')-C(48')	1.429(9)
C(22)-C(23)	1.550(8)		
C(23)-C(24)	1.527(7)		

O(52)-S(1)-O(51)	111.8(3)	N(12)-C(18')-C(17')	122.8(7)
O(52)-S(1)-O(53)	110.6(3)	C(11')-O(21)-C(14)	118.0(4)
O(51)-S(1)-O(53)	108.0(2)	C(15')-O(22)-C(11')	116.6(5)
O(52)-S(1)-O(54)	108.3(3)	C(28')-N(22)-C(13)	119.4(6)
O(51)-S(1)-O(54)	108.5(3)	N(11)-C(21)-C(22)	111.9(5)
O(53)-S(1)-O(54)	109.7(3)	N(11)-C(21)-C(26)	111.3(5)
O(63)-S(2)-O(61)	110.9(3)	C(22)-C(21)-C(26)	110.3(4)
O(63)-S(2)-O(64)	111.2(3)	C(21)-C(22)-C(23)	111.8(5)
O(61)-S(2)-O(64)	108.9(2)	N(12)-C(23)-C(24)	110.0(5)
O(63)-S(2)-O(62)	107.3(3)	N(12)-C(23)-C(22)	108.7(5)
O(61)-S(2)-O(62)	108.2(2)	C(24)-C(23)-C(22)	111.2(5)
O(64)-S(2)-O(62)	110.3(2)	O(11)-C(24)-C(25)	106.9(5)
O(74)-S(3)-O(71)	106.5(4)	O(11)-C(24)-C(23)	104.8(4)
O(74)-S(3)-O(72)	106.6(4)	C(25)-C(24)-C(23)	113.3(5)
O(71)-S(3)-O(72)	114.0(4)	O(13)-C(25)-C(24)	108.3(4)
O(74)-S(3)-O(73)	107.5(4)	O(13)-C(25)-C(26)	108.5(5)
O(71)-S(3)-O(73)	109.9(5)	C(24)-C(25)-C(26)	113.8(5)
O(72)-S(3)-O(73)	111.9(5)	O(14)-C(26)-C(25)	110.2(5)
O(84)-S(4)-O(83)	111.5(3)	O(14)-C(26)-C(21)	109.5(4)
O(84)-S(4)-O(81)	109.8(3)	C(25)-C(26)-C(21)	107.6(5)
O(83)-S(4)-O(81)	111.4(4)	O(11)-C(21')-O(12)	112.4(4)
O(84)-S(4)-O(82)	109.9(3)	O(11)-C(21')-C(22')	108.0(5)
O(83)-S(4)-O(82)	107.9(3)	O(12)-C(21')-C(22')	112.1(5)
O(81)-S(4)-O(82)	106.3(3)	N(13)-C(22')-C(21')	111.7(5)
O(93)-S(5)-O(94)	109.4(4)	N(13)-C(22')-C(23')	110.8(5)
O(93)-S(5)-O(91)	111.0(4)	C(21')-C(22')-C(23')	108.1(5)
O(94)-S(5)-O(91)	107.3(4)	C(24')-C(23')-C(22')	108.3(6)
O(93)-S(5)-O(92)	103.9(5)	C(25')-C(24')-C(23')	124.6(6)
O(94)-S(5)-O(92)	113.1(5)	C(24')-C(25')-O(12)	122.0(6)
O(91)-S(5)-O(92)	112.2(5)	C(24')-C(25')-C(26')	125.9(6)
C(21')-O(11)-C(24)	118.1(4)	O(12)-C(25')-C(26')	112.1(6)
C(21')-O(12)-C(25')	116.2(5)	C(27')-C(26')-C(25')	127.3(7)
C(18')-N(12)-C(23)	118.7(6)	C(26')-C(27')-C(28')	121.2(7)
N(21)-C(11)-C(12)	110.2(5)	N(22)-C(28')-C(27')	121.9(7)
N(21)-C(11)-C(16)	109.8(5)	C(31')-O(31)-C(34)	117.4(4)
C(12)-C(11)-C(16)	110.6(5)	C(35')-O(32)-C(31')	116.9(5)
C(11)-C(12)-C(13)	111.5(5)	C(48')-N(32)-C(33)	119.5(6)
N(22)-C(13)-C(14)	111.0(4)	N(31)-C(31)-C(32)	109.3(4)
N(22)-C(13)-C(12)	108.0(5)	N(31)-C(31)-C(36)	111.4(5)
C(14)-C(13)-C(12)	111.0(5)	C(32)-C(31)-C(36)	109.4(4)
O(21)-C(14)-C(13)	106.7(5)	C(33)-C(32)-C(31)	109.5(5)
O(21)-C(14)-C(15)	108.9(5)	N(32)-C(33)-C(32)	107.7(5)
C(13)-C(14)-C(15)	113.1(5)	N(32)-C(33)-C(34)	108.4(4)
O(23)-C(15)-C(16)	111.9(5)	C(32)-C(33)-C(34)	113.0(4)
O(23)-C(15)-C(14)	105.7(5)	O(31)-C(34)-C(35)	110.0(4)
C(16)-C(15)-C(14)	114.2(5)	O(31)-C(34)-C(33)	105.3(4)
O(24)-C(16)-C(15)	111.3(5)	C(35)-C(34)-C(33)	111.4(4)
O(24)-C(16)-C(11)	111.1(4)	O(33)-C(35)-C(36)	109.6(4)
C(15)-C(16)-C(11)	110.3(5)	O(33)-C(35)-C(34)	106.0(4)
O(21)-C(11')-O(22)	112.0(4)	C(36)-C(35)-C(34)	115.7(4)
O(21)-C(11')-C(12')	107.9(5)	O(34)-C(36)-C(35)	110.4(4)
O(22)-C(11')-C(12')	110.7(5)	O(34)-C(36)-C(31)	108.0(4)
N(23)-C(12')-C(13')	111.2(5)	C(35)-C(36)-C(31)	107.8(4)
N(23)-C(12')-C(11')	112.1(5)	O(32)-C(31')-O(31)	111.4(4)
C(13')-C(12')-C(11')	109.1(5)	O(32)-C(31')-C(32')	111.5(5)
C(14')-C(13')-C(12')	109.0(5)	O(31)-C(31')-C(32')	107.8(5)
C(15')-C(14')-C(13')	123.2(6)	N(33)-C(32')-C(31')	110.5(5)
C(14')-C(15')-O(22)	122.7(6)	N(33)-C(32')-C(33')	110.9(5)
C(14')-C(15')-C(16')	124.0(7)	C(31')-C(32')-C(33')	108.4(5)
O(22)-C(15')-C(16')	113.3(6)	C(34')-C(33')-C(32')	108.5(6)
C(17')-C(16')-C(15')	128.9(7)	C(35')-C(34')-C(33')	121.1(6)
C(16')-C(17')-C(18')	123.2(7)	C(34')-C(35')-O(32)	124.1(6)

C(34')-C(35')-C(36')	120.6(6)	C(46)-C(45)-C(44)	114.1(5)
O(32)-C(35')-C(36')	115.3(6)	O(44)-C(46)-C(45)	111.4(5)
C(37')-C(36')-C(35')	125.7(7)	O(44)-C(46)-C(41)	110.5(4)
C(36')-C(37')-C(38')	120.7(7)	C(45)-C(46)-C(41)	109.9(5)
N(42)-C(38')-C(37')	124.1(7)	O(41)-C(41')-O(42)	109.4(4)
C(44)-O(41)-C(41')	116.5(4)	O(41)-C(41')-C(42')	107.2(4)
C(45')-O(42)-C(41')	117.0(5)	O(42)-C(41')-C(42')	111.0(5)
C(38')-N(42)-C(43)	118.4(6)	N(43)-C(42')-C(41')	110.7(5)
N(41)-C(41)-C(42)	109.9(5)	N(43)-C(42')-C(43')	110.5(5)
N(41)-C(41)-C(46)	109.6(5)	C(41')-C(42')-C(43')	110.2(5)
C(42)-C(41)-C(46)	110.1(5)	C(44')-C(43')-C(42')	109.5(6)
C(43)-C(42)-C(41)	112.5(5)	C(45')-C(44')-C(43')	121.4(6)
N(42)-C(43)-C(42)	109.2(5)	C(44')-C(45')-O(42)	124.3(6)
N(42)-C(43)-C(44)	109.9(5)	C(44')-C(45')-C(46')	122.4(7)
C(42)-C(43)-C(44)	111.9(5)	O(42)-C(45')-C(46')	113.3(6)
O(41)-C(44)-C(43)	108.3(5)	C(47')-C(46')-C(45')	126.5(7)
O(41)-C(44)-C(45)	108.3(5)	C(46')-C(47')-C(48')	120.8(7)
C(43)-C(44)-C(45)	111.8(5)	N(32)-C(48')-C(47')	121.8(7)
O(43)-C(45)-C(46)	110.5(5)		
O(43)-C(45)-C(44)	105.8(4)		

Table 6. Torsion angles [°] for C56 H118 N13 O47 S5.

N(21)-C(11)-C(12)-C(13) 178.0(5)	C(23)-C(24)-C(25)-O(13) 169.6(5)
C(16)-C(11)-C(12)-C(13) -60.4(6)	O(11)-C(24)-C(25)-C(26) 163.7(4)
C(11)-C(12)-C(13)-N(22) 178.7(4)	C(23)-C(24)-C(25)-C(26) 48.8(7)
C(11)-C(12)-C(13)-C(14) 56.8(6)	O(13)-C(25)-C(26)-O(14) 64.7(6)
N(22)-C(13)-C(14)-O(21) 70.8(6)	C(24)-C(25)-C(26)-O(14) -174.7(4)
C(12)-C(13)-C(14)-O(21) -169.1(5)	O(13)-C(25)-C(26)-C(21) -176.0(5)
N(22)-C(13)-C(14)-C(15) -169.4(5)	C(24)-C(25)-C(26)-C(21) -55.4(6)
C(12)-C(13)-C(14)-C(15) -49.3(7)	N(11)-C(21)-C(26)-O(14) -53.2(7)
O(21)-C(14)-C(15)-O(23) -70.2(6)	C(22)-C(21)-C(26)-O(14) -178.0(5)
C(13)-C(14)-C(15)-O(23) 171.3(5)	N(11)-C(21)-C(26)-C(25) -172.9(5)
O(21)-C(14)-C(15)-C(16) 166.4(4)	C(22)-C(21)-C(26)-C(25) 62.2(7)
C(13)-C(14)-C(15)-C(16) 47.9(7)	C(24)-O(11)-C(21')-O(12) 82.6(6)
O(23)-C(15)-C(16)-O(24) 66.0(6)	C(24)-O(11)-C(21')-C(22') -153.2(5)
C(14)-C(15)-C(16)-O(24) -173.9(4)	C(25')-O(12)-C(21')-O(11) 82.2(6)
O(23)-C(15)-C(16)-C(11) -170.2(5)	C(25')-O(12)-C(21')-C(22') -39.6(6)
C(14)-C(15)-C(16)-C(11) -50.1(6)	O(11)-C(21')-C(22')-N(13) 59.1(6)
N(21)-C(11)-C(16)-O(24) -57.8(6)	O(12)-C(21')-C(22')-N(13) -176.6(4)
C(12)-C(11)-C(16)-O(24) -179.6(5)	O(11)-C(21')-C(22')-C(23') -63.0(6)
N(21)-C(11)-C(16)-C(15) 178.3(5)	O(12)-C(21')-C(22')-C(23') 61.3(6)
C(12)-C(11)-C(16)-C(15) 56.5(6)	N(13)-C(22')-C(23')-C(24') -172.0(5)
O(21)-C(11')-C(12')-N(23) 62.3(6)	C(21')-C(22')-C(23')-C(24') -49.4(6)
O(22)-C(11')-C(12')-N(23) -174.8(4)	C(22')-C(23')-C(24')-C(25') 20.9(9)
O(21)-C(11')-C(12')-C(13') -61.3(6)	C(23')-C(24')-C(25')-O(12) 1.8(9)
O(22)-C(11')-C(12')-C(13') 61.6(6)	C(23')-C(24')-C(25')-C(26') -176.9(6)
N(23)-C(12')-C(13')-C(14') -173.7(5)	C(21')-O(12)-C(25')-C(24') 7.6(7)
C(11')-C(12')-C(13')-C(14') -49.6(6)	C(21')-O(12)-C(25')-C(26') -173.5(4)
C(12')-C(13')-C(14')-C(15') 19.4(8)	C(24')-C(25')-C(26')-C(27') -163.7(6)
C(13')-C(14')-C(15')-O(22) 3.1(9)	O(12)-C(25')-C(26')-C(27') 17.5(8)
C(13')-C(14')-C(15')-C(16') -177.0(5)	C(25')-C(26')-C(27')-C(28') 176.1(5)
C(14')-C(15')-C(16')-C(17') -167.0(6)	C(13)-N(22)-C(28')-C(27') -179.1(5)
O(22)-C(15')-C(16')-C(17') 12.8(8)	C(26')-C(27')-C(28')-N(22) -171.7(5)
C(15')-C(16')-C(17')-C(18') 177.5(5)	N(31)-C(31)-C(32)-C(33) 174.3(4)
C(23)-N(12)-C(18')-C(17') 179.1(5)	C(36)-C(31)-C(32)-C(33) -63.5(6)
C(16')-C(17')-C(18')-N(12) -170.7(5)	C(48')-N(32)-C(33)-C(32) 141.0(5)
O(22)-C(11')-O(21)-C(14) 86.7(6)	C(48')-N(32)-C(33)-C(34) -96.5(6)
C(12')-C(11')-O(21)-C(14) -151.2(5)	C(31)-C(32)-C(33)-N(32) 174.0(4)
C(13)-C(14)-O(21)-C(11') -141.0(5)	C(31)-C(32)-C(33)-C(34) 54.3(6)
C(15)-C(14)-O(21)-C(11') 96.6(5)	C(31')-O(31)-C(34)-C(35) 96.3(5)
C(14')-C(15')-O(22)-C(11') 7.6(8)	C(31')-O(31)-C(34)-C(33) -143.6(5)
C(16')-C(15')-O(22)-C(11') -172.3(4)	N(32)-C(33)-C(34)-O(31) 76.1(5)
O(21)-C(11')-O(22)-C(15') 80.7(6)	C(32)-C(33)-C(34)-O(31) -164.7(5)
C(12')-C(11')-O(22)-C(15') -39.7(6)	N(32)-C(33)-C(34)-C(35) -164.7(5)
C(14)-C(13)-N(22)-C(28') -93.2(6)	C(32)-C(33)-C(34)-C(35) -45.4(7)
C(12)-C(13)-N(22)-C(28') 144.9(5)	O(31)-C(34)-C(35)-O(33) -74.7(5)
N(11)-C(21)-C(22)-C(23) 173.1(5)	C(33)-C(34)-C(35)-O(33) 168.9(4)
C(26)-C(21)-C(22)-C(23) -62.4(7)	O(31)-C(34)-C(35)-C(36) 163.6(4)
C(18')-N(12)-C(23)-C(24) -94.6(6)	C(33)-C(34)-C(35)-C(36) 47.2(6)
C(18')-N(12)-C(23)-C(22) 143.5(5)	O(33)-C(35)-C(36)-O(34) 66.6(6)
C(21)-C(22)-C(23)-N(12) 174.2(5)	C(34)-C(35)-C(36)-O(34) -173.6(4)
C(21)-C(22)-C(23)-C(24) 53.0(7)	O(33)-C(35)-C(36)-C(31) -175.7(4)
C(21')-O(11)-C(24)-C(25) 95.8(5)	C(34)-C(35)-C(36)-C(31) -55.9(6)
C(21')-O(11)-C(24)-C(23) -143.7(5)	N(31)-C(31)-C(36)-O(34) -57.1(6)
N(12)-C(23)-C(24)-O(11) 78.1(6)	C(32)-C(31)-C(36)-O(34) -178.0(4)
C(22)-C(23)-C(24)-O(11) -161.5(5)	N(31)-C(31)-C(36)-C(35) -176.3(5)
N(12)-C(23)-C(24)-C(25) -165.8(5)	C(32)-C(31)-C(36)-C(35) 62.8(6)
C(22)-C(23)-C(24)-C(25) -45.3(7)	C(35')-O(32)-C(31')-O(31) 81.7(6)
O(11)-C(24)-C(25)-O(13) -75.5(5)	C(35')-O(32)-C(31')-C(32') -38.7(6)

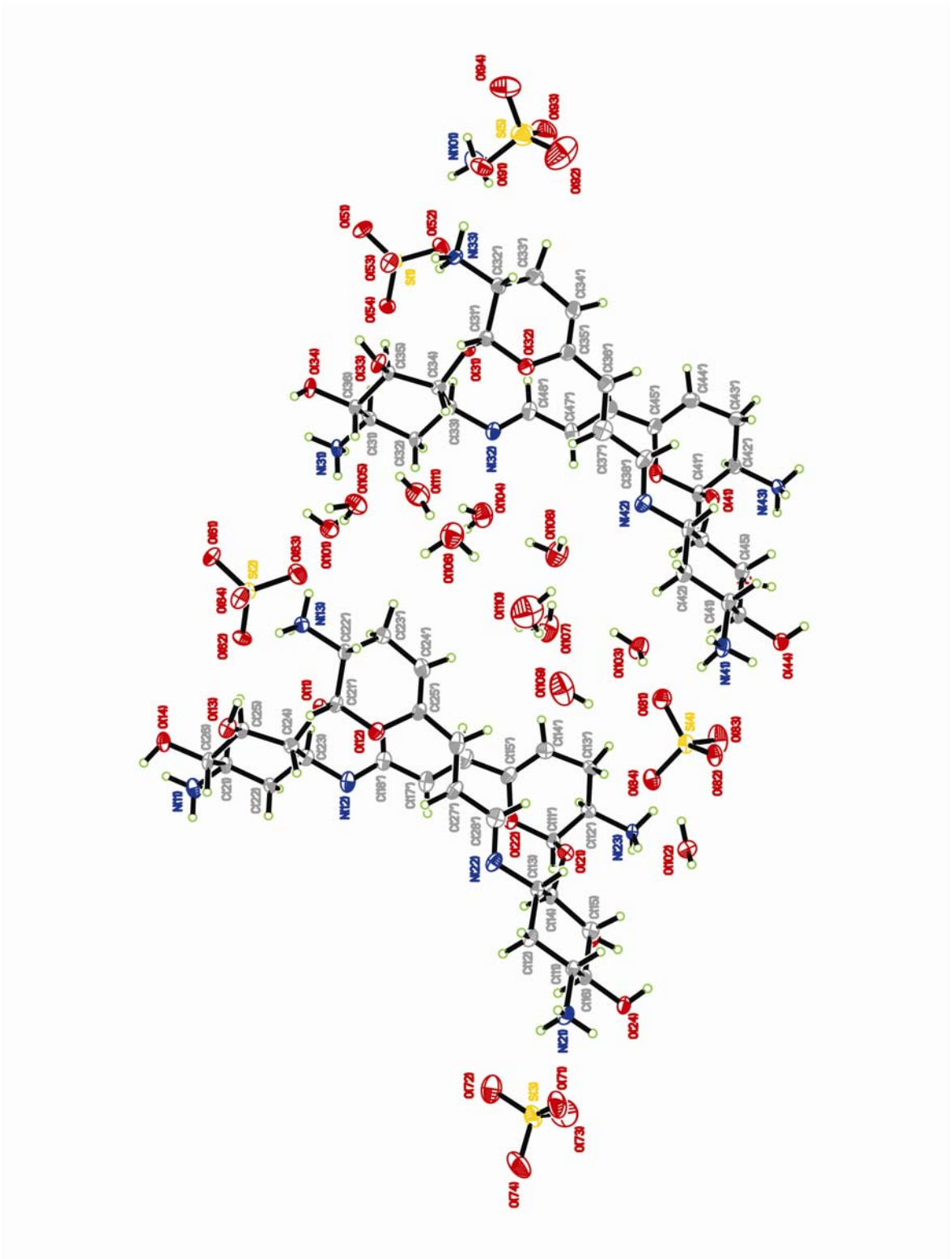
C(34)-O(31)-C(31')-O(32) 81.1(6)	O(41)-C(44)-C(45)-C(46) 168.6(4)
C(34)-O(31)-C(31')-C(32') -156.3(5)	C(43)-C(44)-C(45)-C(46) 49.3(7)
O(32)-C(31')-C(32')-N(33) -176.8(4)	O(43)-C(45)-C(46)-O(44) 65.9(6)
O(31)-C(31')-C(32')-N(33) 60.7(6)	C(44)-C(45)-C(46)-O(44) -175.0(4)
O(32)-C(31')-C(32')-C(33') 61.5(6)	O(43)-C(45)-C(46)-C(41) -171.2(5)
O(31)-C(31')-C(32')-C(33') -61.0(6)	C(44)-C(45)-C(46)-C(41) -52.2(6)
N(33)-C(32')-C(33')-C(34') -173.1(5)	N(41)-C(41)-C(46)-O(44) -59.7(6)
C(31')-C(32')-C(33')-C(34') -51.6(7)	C(42)-C(41)-C(46)-O(44) 179.3(5)
C(32')-C(33')-C(34')-C(35') 23.0(8)	N(41)-C(41)-C(46)-C(45) 177.0(5)
C(33')-C(34')-C(35')-O(32) 0.4(10)	C(42)-C(41)-C(46)-C(45) 56.0(6)
C(33')-C(34')-C(35')-C(36') -178.8(6)	C(44)-O(41)-C(41')-O(42) 92.7(6)
C(31')-O(32)-C(35')-C(34') 7.2(8)	C(44)-O(41)-C(41')-C(42') -146.8(5)
C(31')-O(32)-C(35')-C(36') -173.5(5)	C(45')-O(42)-C(41')-O(41) 81.6(6)
C(34')-C(35')-C(36')-C(37') -164.5(6)	C(45')-O(42)-C(41')-C(42') -36.6(6)
O(32)-C(35')-C(36')-C(37') 16.1(8)	O(41)-C(41')-C(42')-N(43) 61.8(6)
C(35')-C(36')-C(37')-C(38') 178.5(5)	O(42)-C(41')-C(42')-N(43) -178.7(4)
C(36')-C(37')-C(38')-N(42) -169.2(6)	O(41)-C(41')-C(42')-C(43') -60.8(6)
C(37')-C(38')-N(42)-C(43) -179.2(5)	O(42)-C(41')-C(42')-C(43') 58.7(6)
N(41)-C(41)-C(42)-C(43) 179.9(5)	N(43)-C(42')-C(43')-C(44') -172.2(5)
C(46)-C(41)-C(42)-C(43) -59.3(6)	C(41')-C(42')-C(43')-C(44') -49.5(7)
C(38')-N(42)-C(43)-C(42) 145.4(5)	C(42')-C(43')-C(44')-C(45') 20.9(9)
C(38')-N(42)-C(43)-C(44) -91.5(6)	C(43')-C(44')-C(45')-O(42) 1.7(10)
C(41)-C(42)-C(43)-N(42) 178.1(4)	C(43')-C(44')-C(45')-C(46') 179.4(6)
C(41)-C(42)-C(43)-C(44) 56.2(6)	C(41')-O(42)-C(45')-C(44') 6.5(9)
C(41')-O(41)-C(44)-C(43) -144.7(5)	C(41')-O(42)-C(45')-C(46') -171.5(4)
C(41')-O(41)-C(44)-C(45) 93.9(5)	C(44')-C(45')-C(46')-C(47') -164.6(6)
N(42)-C(43)-C(44)-O(41) 69.5(6)	O(42)-C(45')-C(46')-C(47') 13.4(8)
C(42)-C(43)-C(44)-O(41) -169.1(5)	C(45')-C(46')-C(47')-C(48') 177.4(5)
N(42)-C(43)-C(44)-C(45) -171.3(5)	C(33)-N(32)-C(48')-C(47') -179.1(5)
C(42)-C(43)-C(44)-C(45) -49.8(7)	C(46')-C(47')-C(48')-N(32) -170.9(5)
O(41)-C(44)-C(45)-O(43) -69.8(5)	
C(43)-C(44)-C(45)-O(43) 170.9(5)	

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C56 H118 N13 O47 S5.

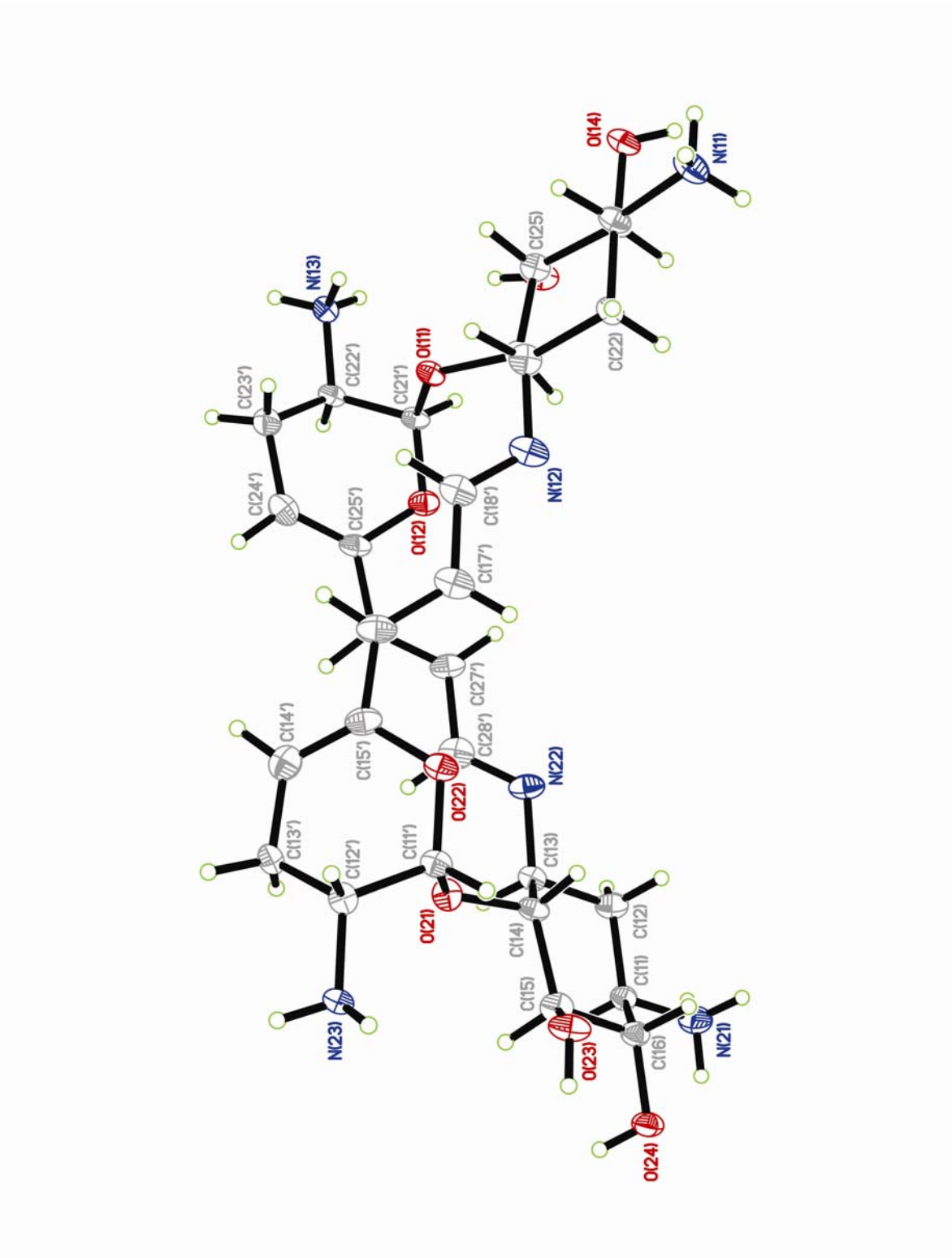
D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
O(14)-H(14)	O(73)#1	0.84	2.15	2.668(7)	119.9
N(11)-H(11A)	O(71)#2	0.91	1.96	2.816(8)	156.7
N(11)-H(11B)	O(93)#3	0.91	1.9	2.778(9)	162.1
N(11)-H(11B)	O(94)#3	0.91	2.43	3.105(9)	131.4
N(11)-H(11C)	O(13)#4	0.91	2.18	2.911(7)	136.8
N(13)-H(13A)	O(101)	0.91	1.98	2.868(7)	165.4
N(13)-H(13B)	O(62)	0.91	1.93	2.817(6)	163.2
N(13)-H(13C)	O(64)#4	0.91	1.99	2.798(6)	147.5
O(23)-H(23)	O(64)#5	0.84	2.05	2.782(6)	146
O(24)-H(24)	O(62)#6	0.84	2.06	2.693(6)	131.6
N(21)-H(21B)	O(14)#7	0.91	2.04	2.865(7)	150
N(21)-H(21C)	O(71)	0.91	2.45	2.993(8)	118.9
N(23)-H(23A)	O(82)#4	0.91	2.04	2.824(7)	144
N(23)-H(23B)	O(61)#5	0.91	1.91	2.803(6)	165.1
N(23)-H(23C)	O(102)	0.91	2.13	2.873(6)	138.1
O(33)-H(33)	O(44)#1	0.84	1.91	2.693(5)	153.6
O(34)-H(34)	O(83)#1	0.84	1.82	2.639(6)	162.8
N(31)-H(31A)	O(105)#4	0.91	1.9	2.807(7)	173.2
N(31)-H(31B)	O(33)#4	0.91	2.23	2.936(6)	133.5
N(31)-H(31C)	O(82)#2	0.91	1.92	2.769(6)	154.9
N(31)-H(31C)	O(83)#2	0.91	2.63	3.150(7)	117
N(33)-H(33A)	O(53)	0.91	1.95	2.764(6)	148.3
N(33)-H(33B)	O(91)	0.91	1.91	2.804(7)	167
N(33)-H(33C)	O(54)#8	0.91	1.9	2.803(6)	169.9
O(43)-H(43G)	O(53)#6	0.84	1.89	2.705(6)	164.3
O(44)-H(44B)	O(54)#7	0.84	1.85	2.663(6)	161.1
N(41)-H(41A)	O(103)#8	0.91	1.85	2.755(7)	173.2
N(41)-H(41B)	O(34)#7	0.91	1.98	2.814(7)	152.2
N(41)-H(41C)	O(81)	0.91	1.94	2.835(7)	167.6
N(41)-H(41C)	O(82)	0.91	2.53	3.131(7)	123.6
N(43)-H(43B)	O(74)#9	0.91	1.86	2.770(8)	175.1
N(43)-H(43C)	O(51)#6	0.91	1.88	2.771(7)	166
O(101)-H(1E)	O(102)#1	0.863(9)	2.03(3)	2.722(7)	137(4)
O(101)-H(1F)	O(111)	0.868(8)	2.12(4)	2.830(8)	138(5)
O(102)-H(2A)	O(84)	0.861(9)	1.88(3)	2.657(6)	149(5)
O(102)-H(2A)	O(83)	0.861(9)	2.62(3)	3.355(8)	144(4)
O(102)-H(2B)	O(61)#6	0.863(9)	1.947(15)	2.777(6)	161(4)
O(103)-H(3A)	O(107)	0.867(9)	1.97(5)	2.765(8)	151(8)
O(103)-H(3B)	O(81)	0.864(9)	1.974(15)	2.829(7)	170(6)
O(104)-H(4A)	O(106)#4	0.86	2.01	2.863(8)	178
O(104)-H(4B)	O(111)	0.86	1.98	2.837(8)	178.1
O(105)-H(5A)	O(63)	0.884(15)	1.97(4)	2.641(6)	132(4)
O(105)-H(5B)	O(101)#8	0.898(15)	2.18(5)	2.749(7)	121(5)
O(106)-H(6B)	O(110)	0.87	2.21	3.082(10)	177.6
O(107)-H(7A)	O(108)	0.88	1.95	2.832(9)	177.8
O(107)-H(7B)	O(110)#4	0.880(15)	2.31(4)	2.794(10)	115(3)
O(108)-H(8B)	O(104)	0.876(15)	1.90(3)	2.743(8)	162(9)
O(109)-H(9A)	O(81)	0.877(15)	2.11(9)	2.880(9)	146(14)
O(109)-H(9B)	O(107)	0.870(15)	1.969(15)	2.814(10)	163(4)
O(110)-H(10A)	O(109)	0.88	2.21	3.089(12)	175.3
O(111)-H(11E)	O(106)	0.864(9)	2.11(3)	2.886(9)	150(5)
N(101)-H(1A)	O(91)	0.906(17)	2.51(4)	3.042(8)	118(3)
N(101)-H(1B)	O(74)#10	0.889(17)	2.16(3)	2.894(10)	139(4)
N(101)-H(1C)	O(94)#4	0.899(17)	2.24(4)	2.853(10)	125(4)
N(101)-H(1D)	O(52)	0.900(17)	2.23(4)	2.730(9)	115(4)

Symmetry transformations used to generate equivalent atoms:

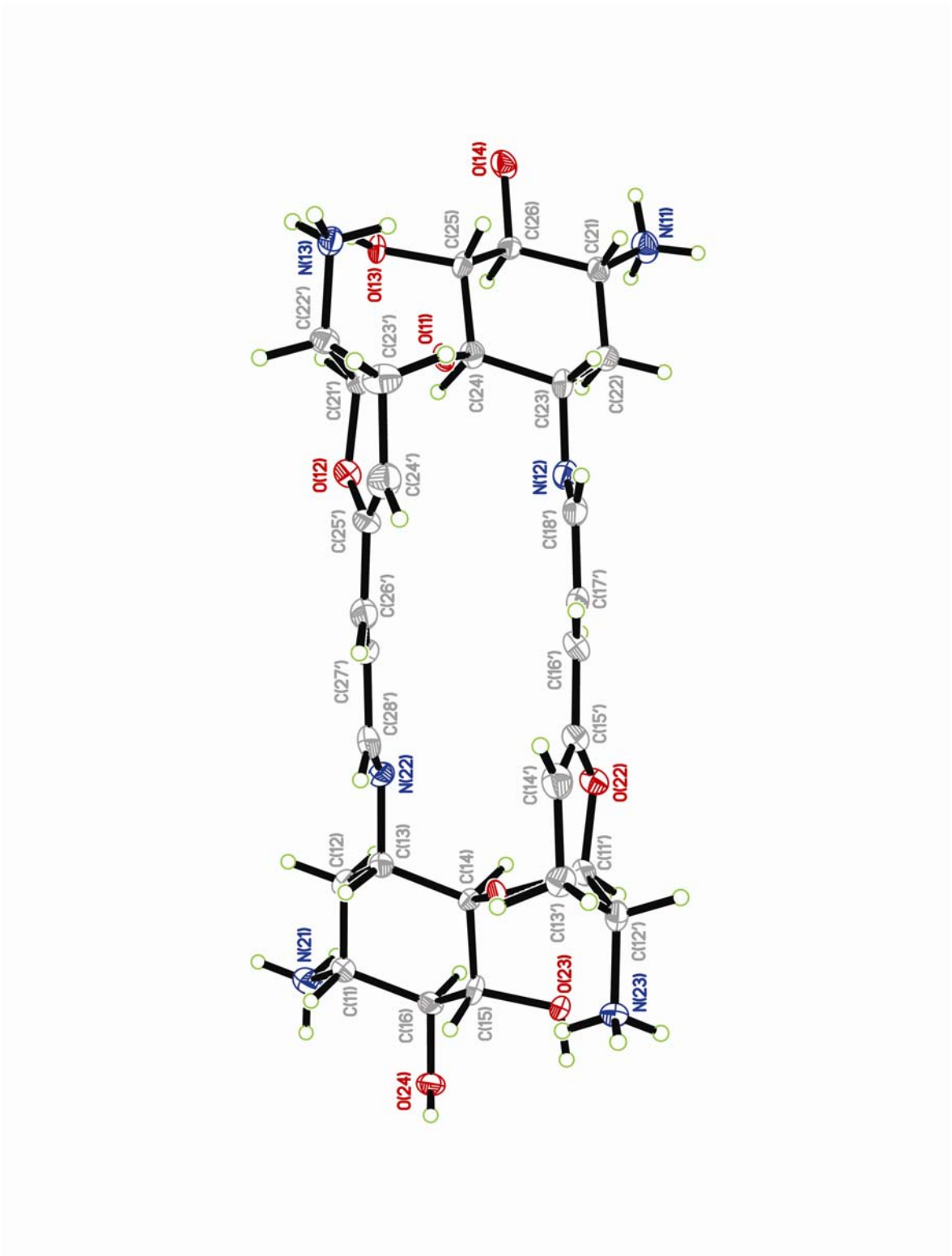
#1 x,y-1,z	#2 x-1,y-1,z	#3 x-1,y,z-1
#4 x-1,y,z	#5 x-1,y+1,z	#6 x,y+1,z
#7 x+1,y+1,z	#8 x+1,y,z	#9 x,y,z+1
#10 x,y-1,z+1		



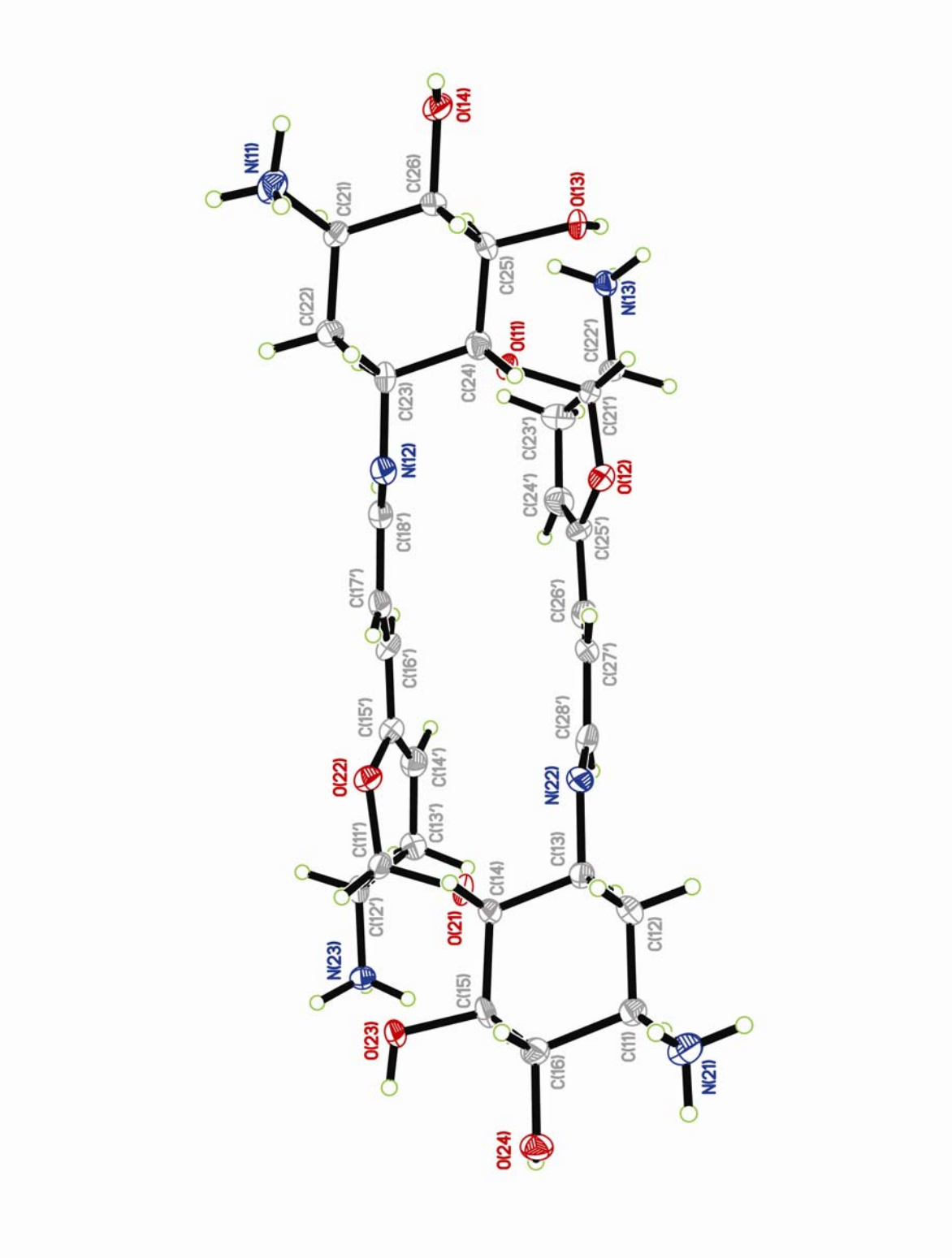
ORTEP view of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



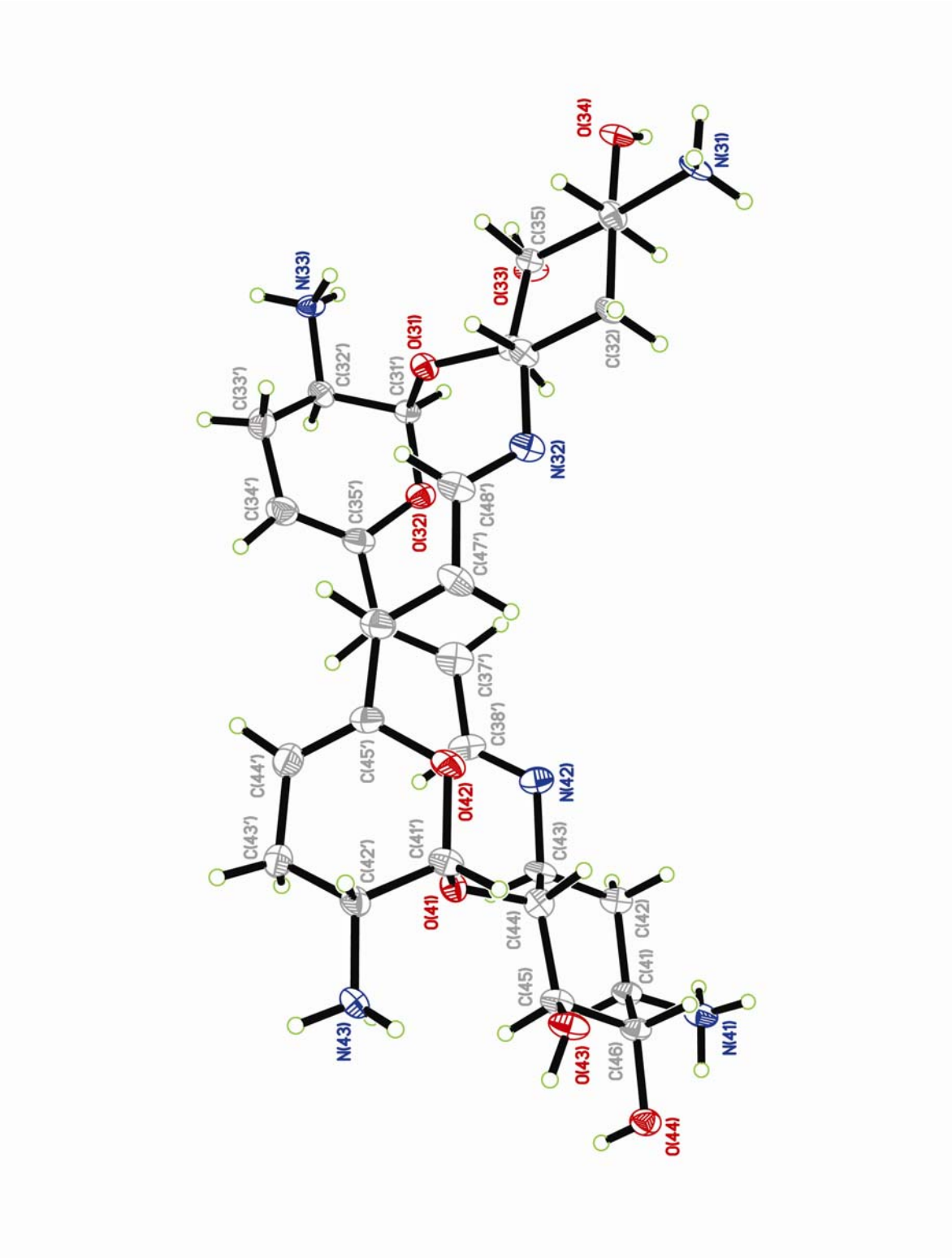
ORTEP side view (molecule A only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



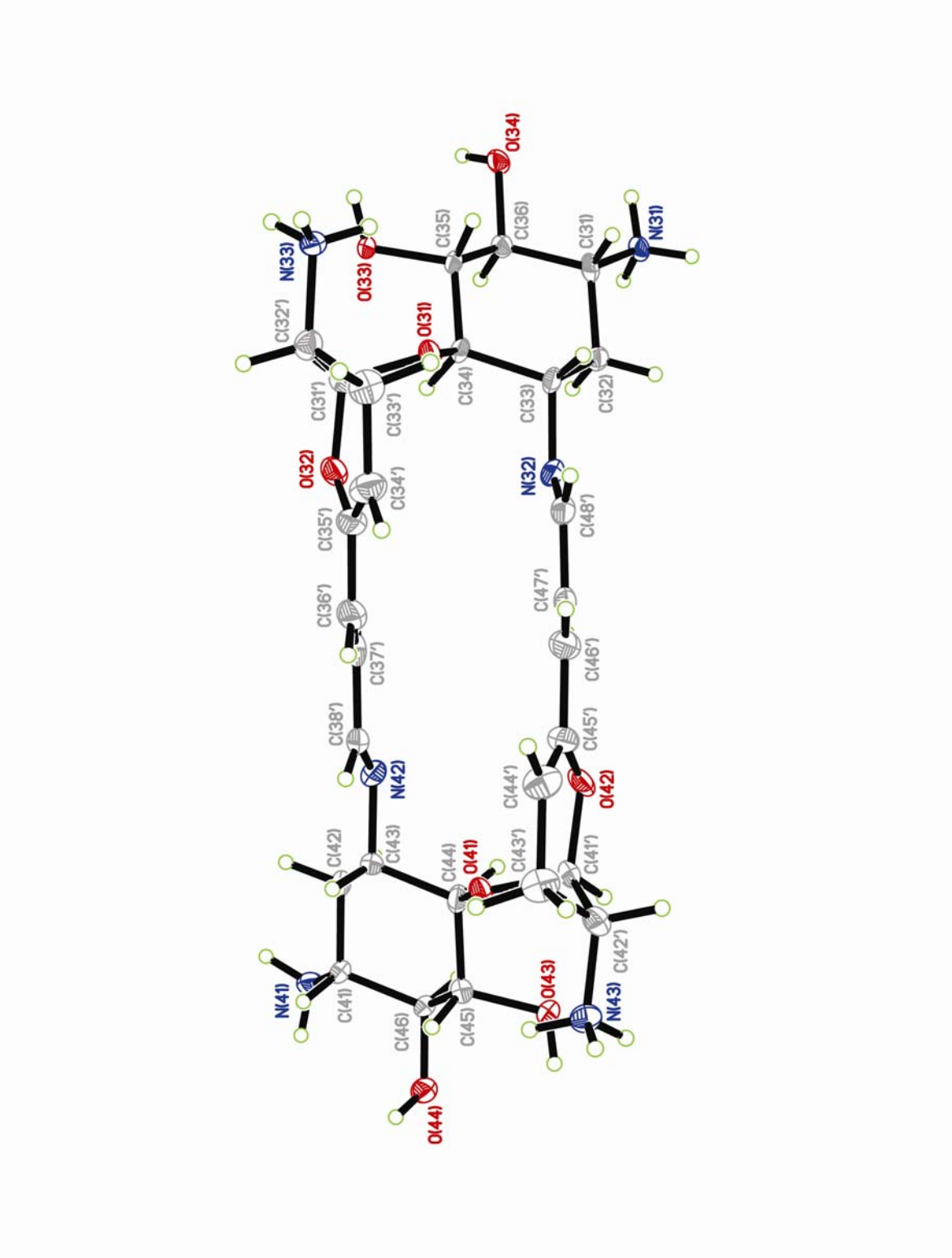
ORTEP top view (molecule A only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



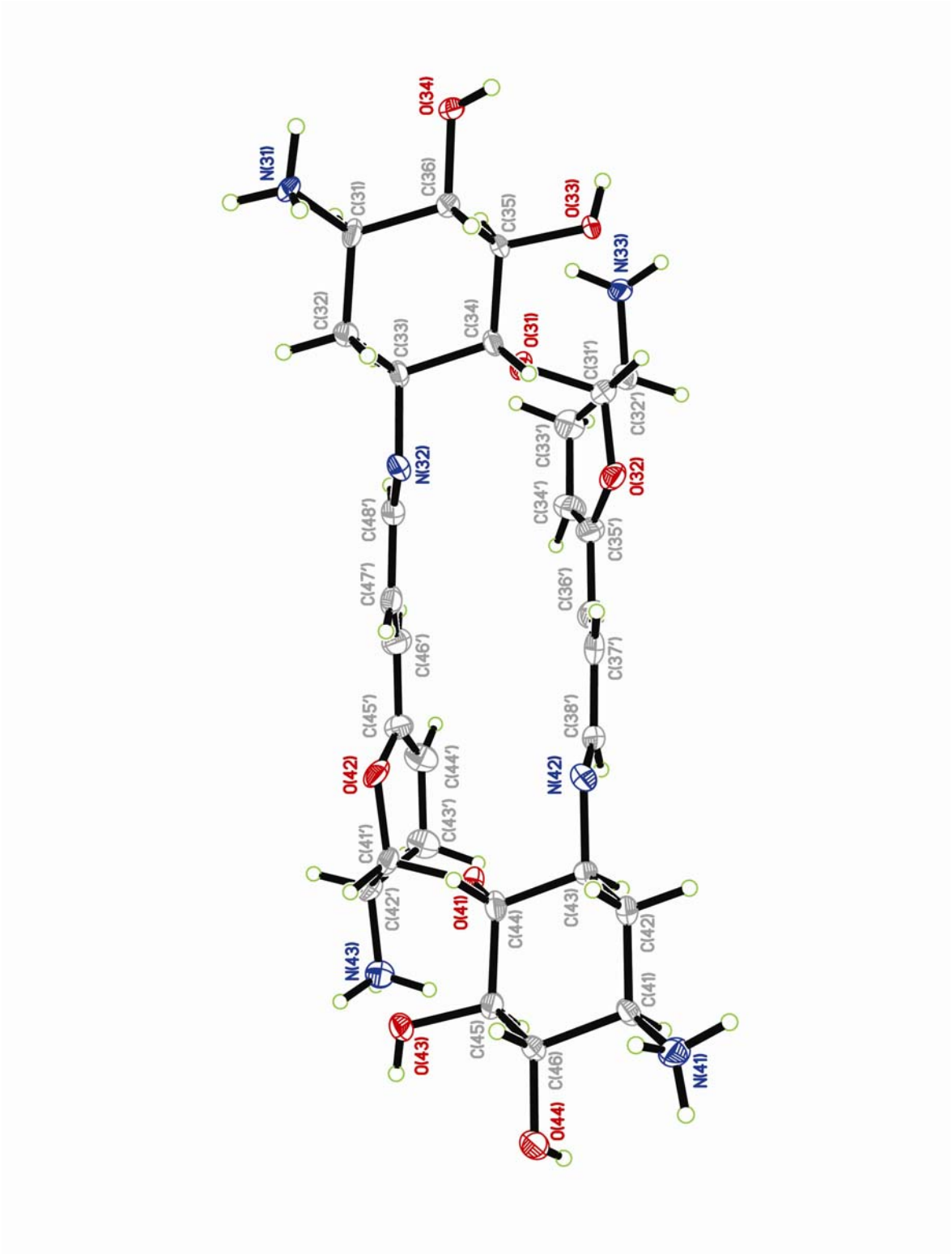
ORTEP bottom view (molecule A only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



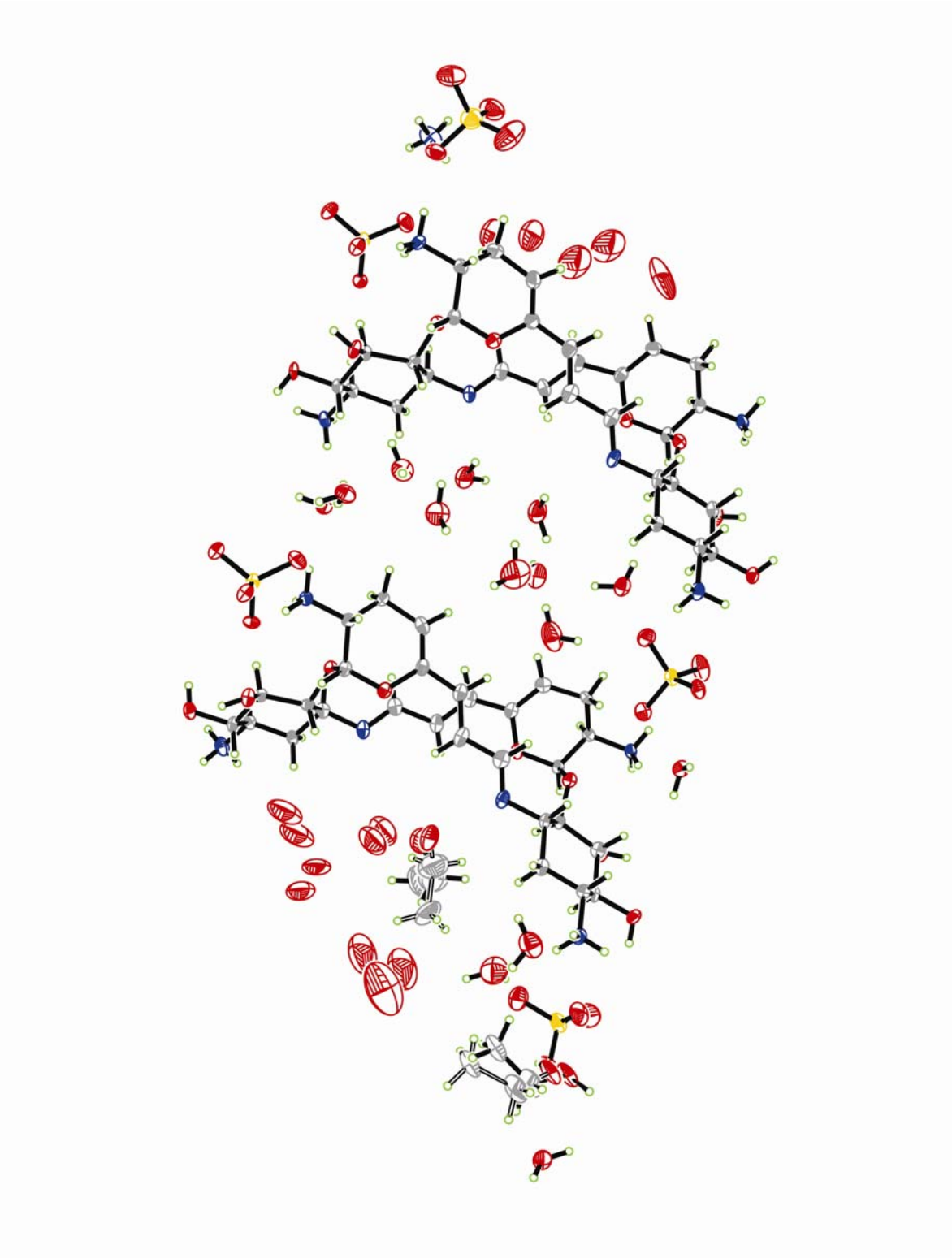
ORTEP side view (molecule B only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP top view (molecule B only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP bottom view (molecule B only) of the C56 H118 N13 O47 S5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.



ORTEP view (speculation based on an attempt to solve the disordered area containig H_2O molecules, C_2H_5O molecules and one NH_4^+ ion) of the C60 H150 N14 O58 S5 of the structure.compound. Ellipsoids drawn at 30% probability level. Hydrogen atoms are represented by sphere of arbitrary size.

REFERENCES

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checkCIF/PLATON (standard)

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: bent70

Bond precision: C-C = 0.0092 A Wavelength=1.54178
Cell: a=6.6138(4) b=16.3922(10) c=23.9598(14)
alpha=101.113(3) beta=92.328(3) gamma=95.176(3)
Temperature: 150 K

	Calculated	Reported
Volume	2534.0(3)	2534.0(3)
Space group	P 1	P1
Hall group	P 1	P 1
Moiety formula	2(C28 H46 N6 O8), 5(O4 S), H4 N, 11(H2 O)	2(C28 H46 N6 O8), 5(O4 S), H4 N, 11(H2 O)
Sum formula	C56 H118 N13 O47 S5	C56 H118 N13 O47 S5
Mr	1885.98	1885.98
Dx,g cm-3	1.236	1.236
Z	1	1
Mu (mm-1)	1.835	1.835
F000	1001.0	1001.0
F000'	1006.26	
h,k,lmax	8,19,29	7,19,28
Nref	9420[18840]	12907
Tmin,Tmax	0.936,0.964	0.502,0.964
Tmin'	0.507	

Correction method= MULTI-SCAN
Data completeness= 1.37/0.69 Theta(max)= 69.170
R(reflections)= 0.0766(9594) wR2(reflections)= 0.1971(12907)
S = 0.969 Npar= 1168

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full Low 0.939

Author Response: Due to geometrical constraints of the instrument and the use of copper radiation, we obtain consistently a data completeness lower than 100% in dependence of the crystal system and the orientation of the mounted crystal, even with appropriate data collection routines. Typical values for data completeness range from 83-92% for triclinic, 85-97% for monoclinic and 85-98% for all other crystal systems. (Note: This comment is routinely included into the CIF-file and can be ignored if the data completeness is satisfactory.)

Alert level B

PLAT420_ALERT_2_B D-H Without Acceptor O111 - H11D ... ?

Author Response: The O111-H11D bond (H2O molecule) is making a weak electrostatic interaction with the main molecule. For N21-H21A (protonated amine) this is due to hydrogen-bonding, with highly disordered solvent as the acceptor (H2O), which is not included in the final model. See PLATON squeeze details in CIF

Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S3

Author Response: Due to minor rotation disorder of the sulfate anion around the sulfur.

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S4

Author Response: Due to minor rotation disorder of the sulfate anion around the sulfur.

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of S5

Author Response: Due to minor rotation disorder of the sulfate anion around the sulfur.

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0092 Ang

Author Response: Low diffraction was observed for this crystal and was especially low for high angles. Many solvent systems were tested for recrystallization. The best crystal was chosen and its size was in the limits of the diffractometer. X-ray measurements were acquired at 150K with optimized radiation exposure time and intensity. The final structure was satisfactory for confirming the desired chemical information.

PLAT420_ALERT_2_C D-H Without Acceptor N21 - H21A ... ?

Author Response: The O111-H11D bond (H2O molecule) is making a weak electrostatic interaction with the main molecule. For N21-H21A (protonated amine) this is due to hydrogen-bonding, with highly disordered solvent as the acceptor (H2O), which is not included in the final model. See PLATON squeeze details in CIF

PLAT480_ALERT_4_C Long H...A H-Bond Reported H31C .. O83 .. 2.63 Ang.

Author Response: These H-Bonds are listed and reported by SHELXTL and they should be considered as weak H-bond interactions (2.2A-3.2A).

PLAT480_ALERT_4_C Long H...A H-Bond Reported H2A .. O83 .. 2.62 Ang.

Author Response: These H-Bonds are listed and reported by SHELXTL and they should be considered as weak H-bond interactions (2.2A-3.2A).

Alert level G

REFLT03_ALERT_4_G WARNING: Large fraction of Friedel related reflns may be needed to determine absolute structure
From the CIF: _diffrn_reflns_theta_max 69.17
From the CIF: _reflns_number_total 12907
Count of symmetry unique reflns 9420
Completeness (_total/calc) 137.02%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 3487
Fraction of Friedel pairs measured 0.370
Are heavy atom types Z>Si present yes
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 39
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained Atom Sites 2
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in CIF .... ?
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.15
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal ..... 0.00300 Deg.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure !

Author Response: The crystal structure has been squeezed with PLATON to remove highly disordered H2O, EtOH and ammonium ion contributions from its solvate structure. Overall, PLATON found a solvent accessible void volume of 473.8 A^3 corresponding to a contribution of 129 electrons per cell. More precisely, this void is estimated to contain 9 molecules of H2O, 2 molecules of EtOH and 1 ammonium ion, which were used as crystallization solvents and crystallization agents ((NH4)2SO4). This speculation is based on an attempt to solve this disordered area of the structure. Considering the solvents and the ammonium ion the physical data should be: Formula moiety: '2(C28 H46 N6 O8), 5(O4 S), 2(H4 N), 20(H2 O), 2(C2 H5 O)' or 'C60 H150 N14 O58 S5' Density: 1.413 g cm-3 Absorption coefficient: 1.988 mm-1 F000: 1152.0

PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
C28 H46 N6 O8
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 3
O4 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 7
O4 S
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 8
H4 N

PLAT791_ALERT_4_G Note: The Model has Chirality at C11 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C11' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C12' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C13 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C14 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C15 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C16 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C21 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C21' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C22' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C23 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C24 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C25 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C26 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C31 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C31' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C32' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C33 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C34 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C35 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C36 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C41 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C41' (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C42' (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C43 (Verify) S
PLAT791_ALERT_4_G Note: The Model has Chirality at C44 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C45 (Verify) R
PLAT791_ALERT_4_G Note: The Model has Chirality at C46 (Verify) S
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 343
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed !

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1 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
41 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
40 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

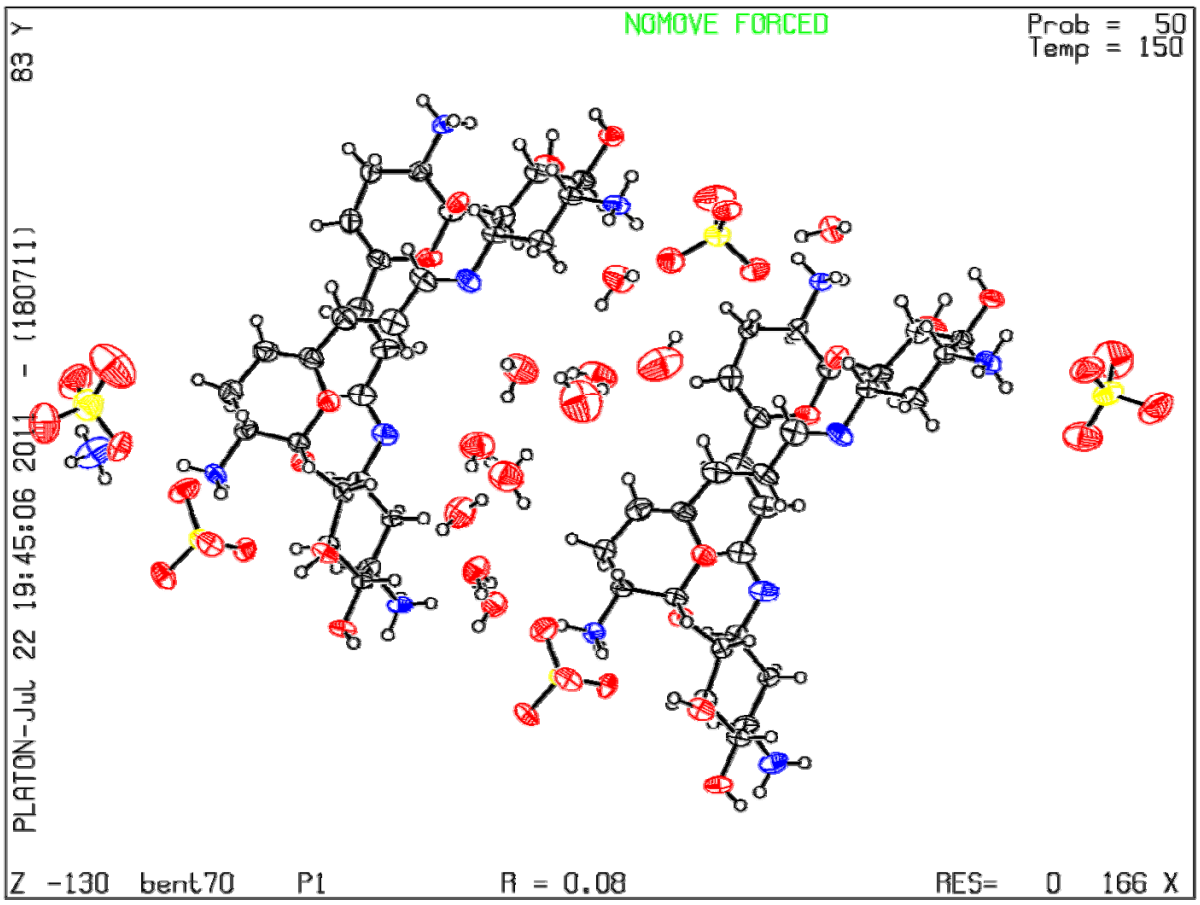
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 18/07/2011; check.def file version of 04/07/2011

Datablock bent70 - ellipsoid plot



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