

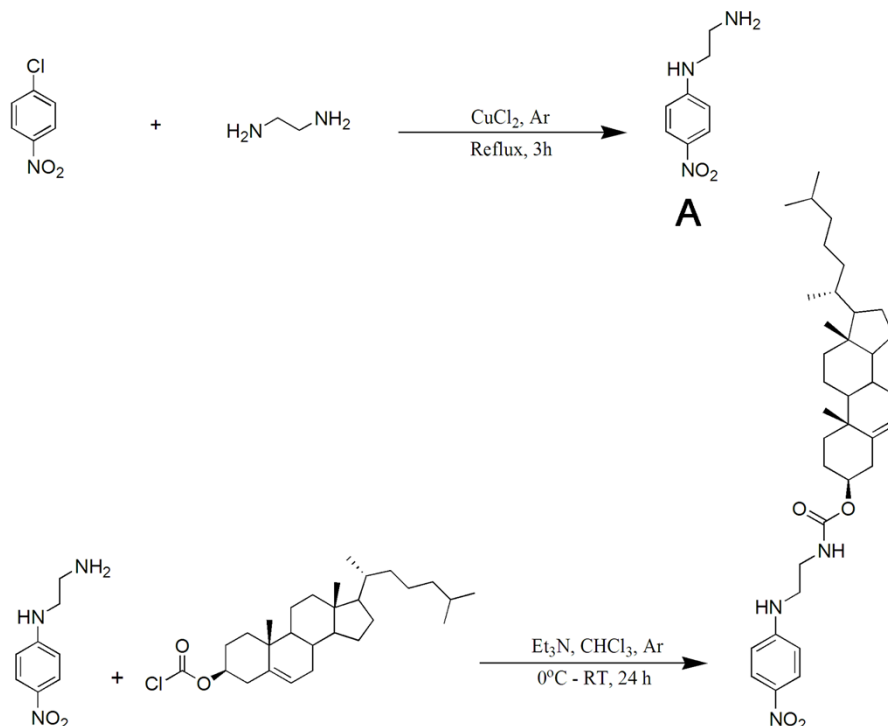
Self-Assembly Patterns of Steroid-Based All-Organic Ferroelectrics: Valuable Insights from the Single-Crystals Derived from Organogel and Solution

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Synthesis of 1:



Synthetic Procedure for A- In a 100 ml round bottomed flask, p-nitrochlorobenzene (24.0 g, 152.32 mmol) was added to a solution of anhydrous CuCl₂ (1.9 g, 14.07 mmol) in 42.8 mL (639.75 mmol) of ethylenediamine and mixture was refluxed for 3 hours under argon atmosphere. After completion of reaction the reaction mixture was cooled and 260 ml of water was added, stirred for 15 minutes, and filtered. Precipitate was recrystallized from boiling water and dried under vacuum to obtain product as orange solid: Yield- 48%. R_f = 0.52 (9:1 CHCl₃/MeOH). Melting point: 150 °C.^a

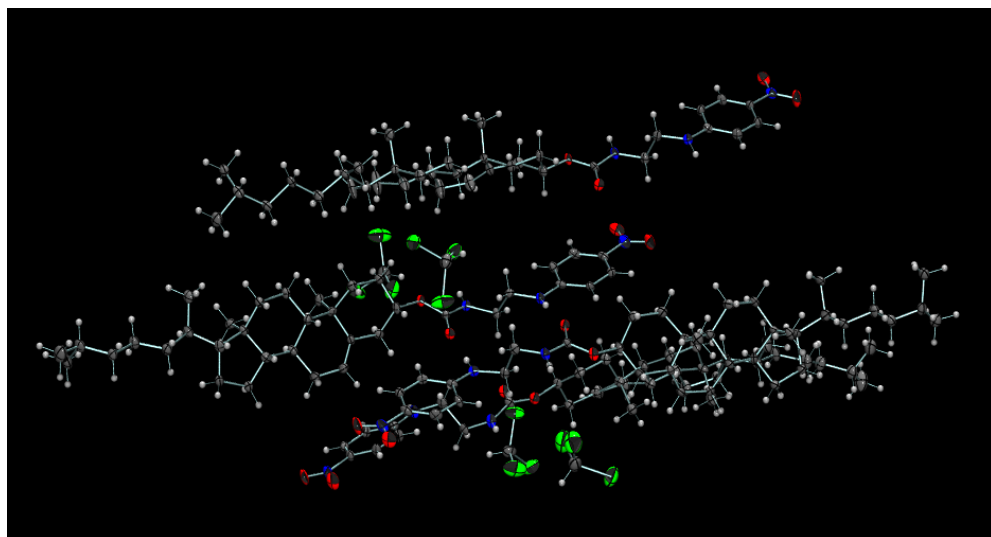
Synthetic Procedure for 1- In a 100 mL round bottomed flask cholesterylchloroformate (2.62 g, 5.83 mmol) was taken in 80.0 ml of dry chloroform and cooled to 0 °C under argon atmosphere. Subsequently **A** (0.95 g, 5.25 mmol) and 1.2 ml of Et₃N was added to this solution and stirred for 24 hours. The reaction mixture was washed with water, dried over NaSO₄ and solvent was evaporated using rotary evaporator. The crude product was purified by washing it with methanol (5 x 30 mL) and dried under vacuum to obtain pure product as yellow solid: Yield- 85%. R_f = 0.684 (9:1 CHCl₃/MeOH). Melting point: 172 °C. ¹H NMR (500 MHz, DMSO-*d*₆, 296 K, TMS): δ = 7.99 (s, 2H, Ar); 7.19-7.31 (br, m, 2H, HN); 6.65 (d, 2H, Ar); 5.33 (s, br, 1H, HC=C); 4.31 (br, m, 1H, CH-O); 3.22 (m, 2H, CH₂); 3.13 (m, 2H, CH₂); 2.25 (m, 2H, CH₂); 1.78-1.97 (m, 5H); 0.97-1.54 (m, 33H); 0.65 (s, 3H, CH₃); ¹³C NMR (125 MHz, DMSO-*d*₆, 296 K, TMS): δ = 154.99, 140.30, 136.44, 126.57, 122.28, 111.30, 73.69, 56.66, 56.17, 50.06, 42.40, 39.44, 38.76, 37.09, 36.60, 36.18, 35.62, 34.67, 31.95, 31.84, 28.34, 28.19, 27.82, 25.26, 24.32, 23.70, 23.06, 22.83, 21.08, 19.44, 19.06, 12.15; FTIR (KBr Pellet): 3421 (ν_{NH}), 3342 (ν_{NH}), 2937

(ν_{CH_2}), 2869 (ν_{CH_3}), 1707 (ν_{CO}), 1605 (ν_{COO}), 1499 (ν_{NO_2}), 1469, 1326, 1259 cm^{-1} . Anal Calcd. For $\text{C}_{36}\text{H}_{55}\text{N}_3\text{O}_4$: C 72.81, H 9.34, N 7.08; Found: C 72.75, H 9.45, N 7.13.

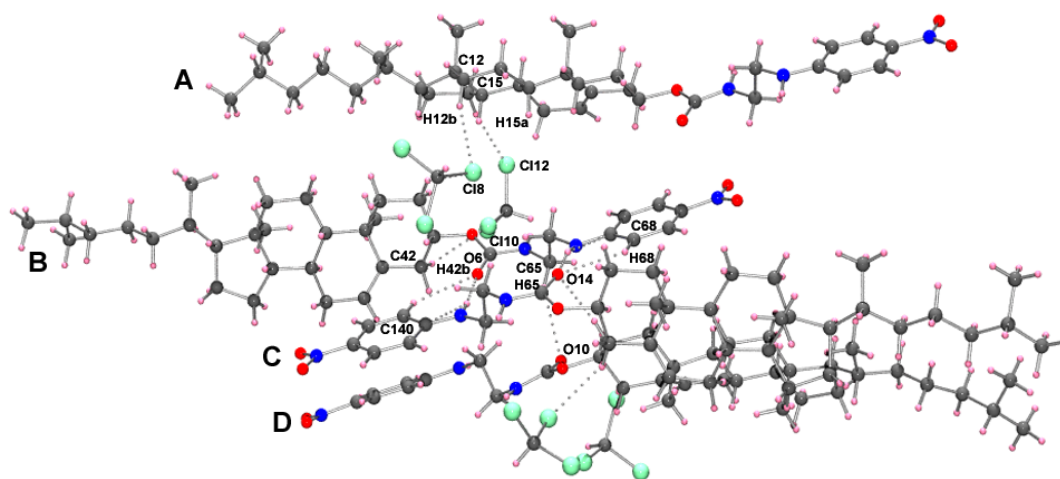
Table-1: Organogelation tests: G_{RT} - Gel at RT, G_{F} - Forms Gel when cooled under fridge, G_{S} - Gel on sonification, G^* - Gel like, S- Solution.

Molecule 1

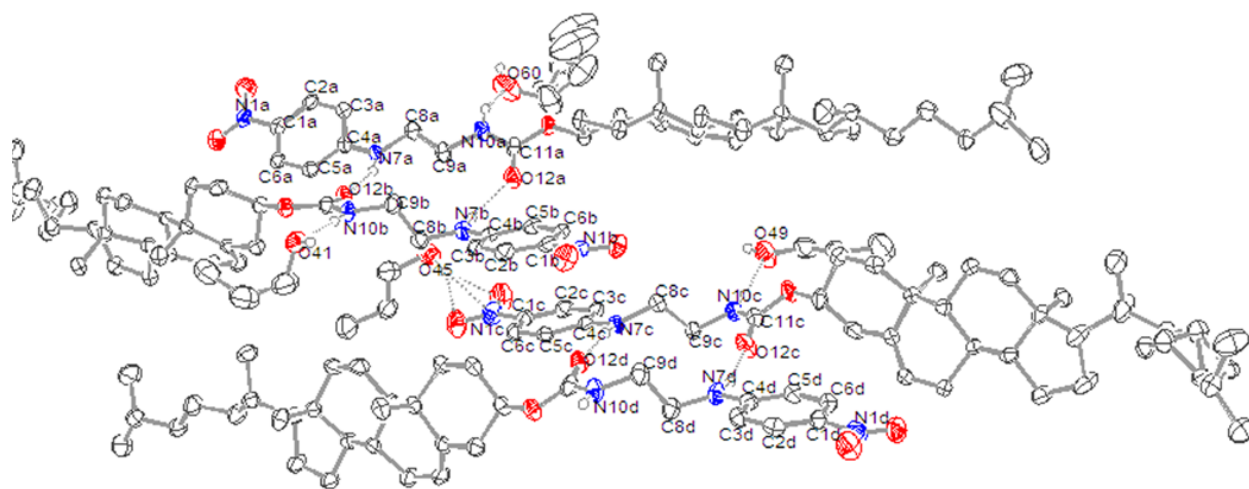
Solvent	2.0 wt%	1.0 wt%	0.5 wt%	0.25 wt%
MeOH		G_{RT}	P	-
CCl_4	G_{F}	G_{F}	G_{F}	S
Acetic Acid	G_{RT}	G_{S}	S	-
THF/MeOH (1:9)	G_{RT}	G_{RT}	G_{F}	G_{F}
$\text{CHCl}_3/\text{MeOH}$ (1:9)	G_{RT}	G_{RT}	G_{F}	G_{F}
$\text{CHCl}_3/\text{n-Hexane}$ (1:9)	G_{RT}	G_{F}	G_{F}	S



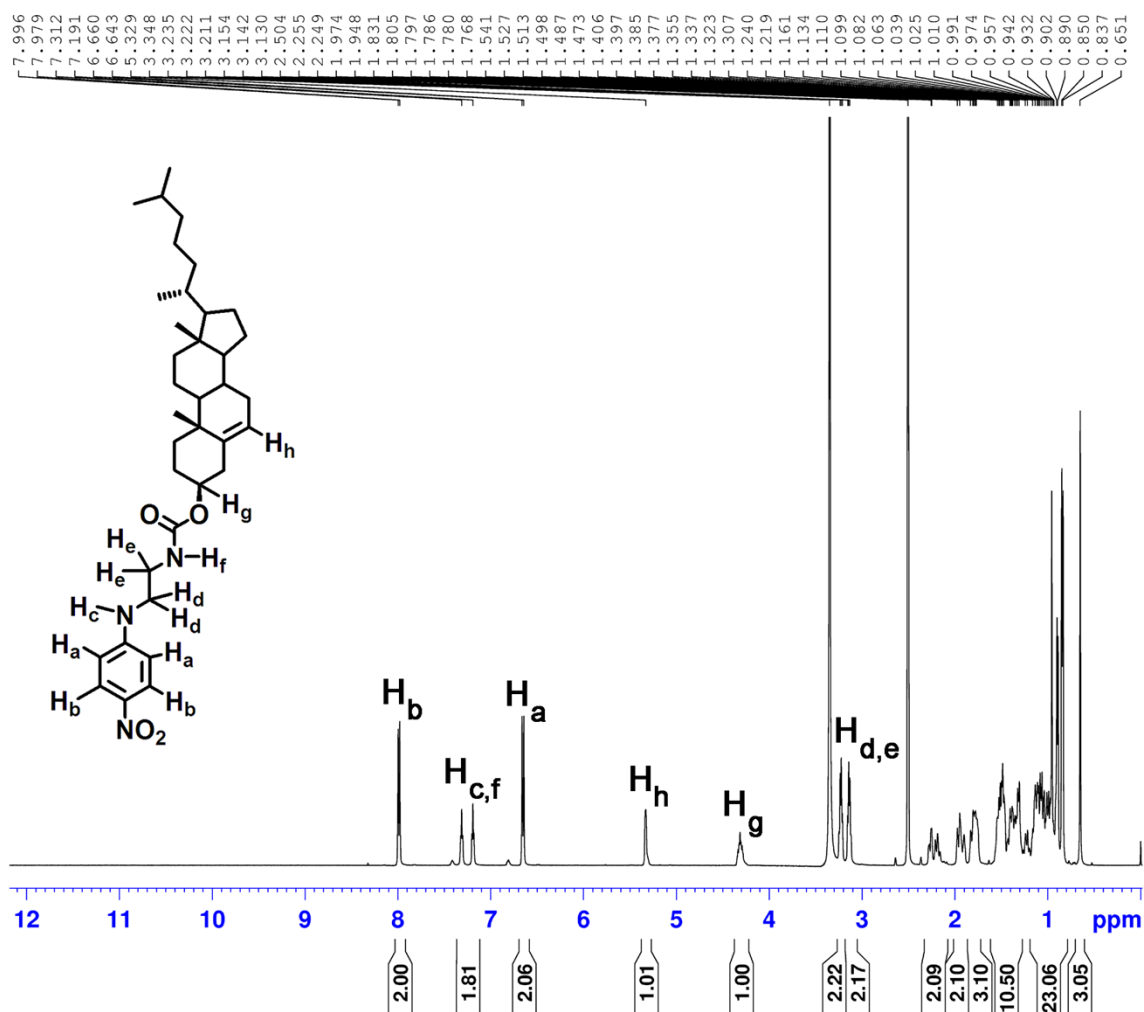
SI 1: ORTEP diagram showing the thermal ellipsoids of **1·Ch** showing the four independent molecules of **1** and the four solvent chloroform molecules.



SI 2: H-bonding pattern of the four independent molecules of **1** with the solvent chloroform molecule.

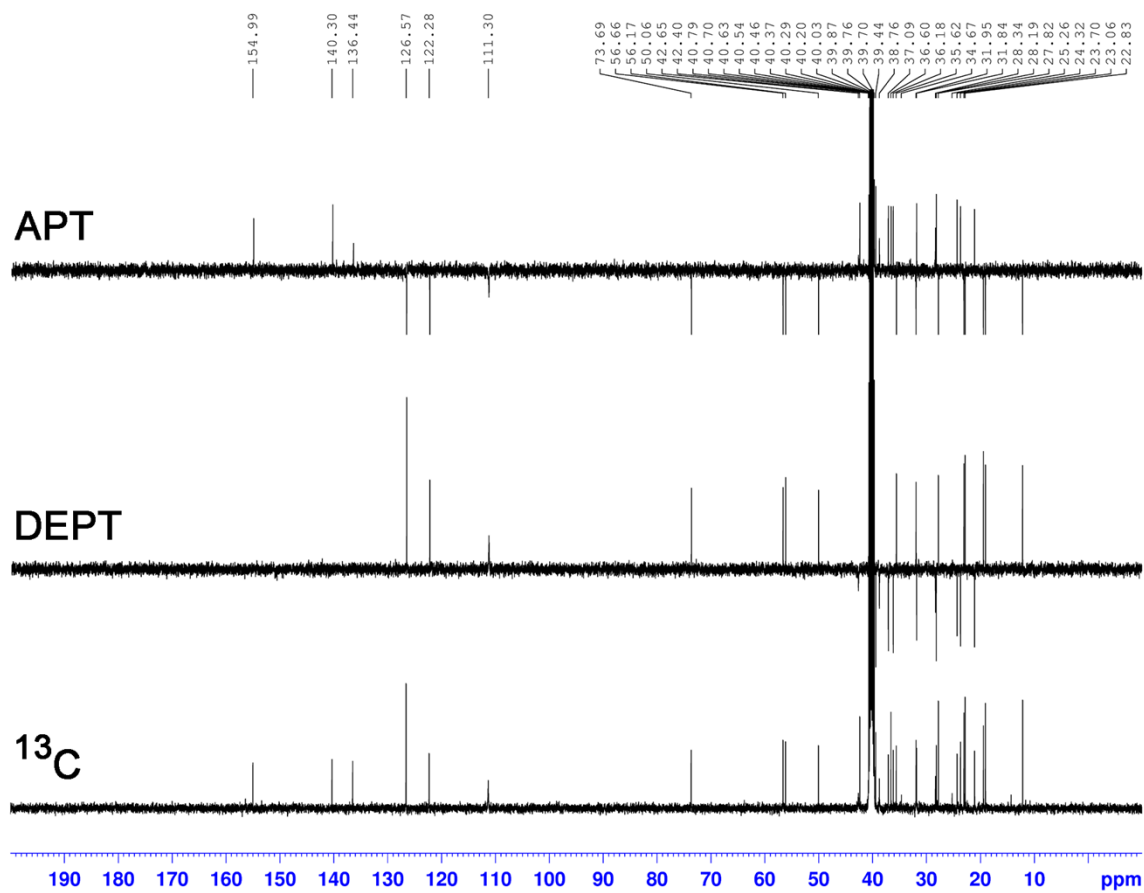


500 MHz ^1H NMR Spectrum of Compound 1:



SI 5: 500 MHz ^1H NMR Spectrum of Compound 1 in $\text{DMSO}-d_6$, 296 K

125 MHz ^{13}C , DEPT-135 and APT NMR Spectra of Compound 1:



SI 6: 125 MHz ^{13}C , DEPT-135 and APT NMR Spectra of Compound 1 in $\text{DMSO}-d_6$

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1·Ch**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
C(1)	9739(4)	9895(4)	4839(2)	24(1)
C(2)	8754(4)	10878(4)	4490(2)	24(1)
C(3)	8153(4)	10415(4)	4189(2)	24(1)
C(4)	8901(4)	9686(4)	3785(2)	20(1)
C(5)	9978(4)	8789(4)	4109(2)	25(1)
C(6)	10541(4)	9160(4)	4479(2)	27(1)
C(7)	10452(5)	7724(5)	4059(2)	43(2)
C(8)	10009(6)	7259(5)	3688(3)	53(2)
C(9)	9083(4)	8199(4)	3261(2)	30(1)
C(10)	8293(4)	9103(4)	3567(2)	24(1)
C(11)	7198(4)	9965(4)	3206(2)	25(1)
C(12)	6640(4)	9424(4)	2940(2)	28(1)
C(13)	7450(4)	8630(4)	2590(2)	20(1)
C(14)	8445(5)	7726(4)	2995(2)	34(1)
C(15)	9097(6)	6828(5)	2661(3)	64(2)
C(16)	8159(5)	6820(5)	2326(3)	53(2)
C(17)	7041(4)	7858(4)	2394(2)	28(1)
C(18)	6245(4)	8347(4)	1867(2)	24(1)
C(19)	5883(5)	7460(4)	1774(2)	32(1)
C(20)	5396(5)	7687(4)	1191(2)	28(1)
C(21)	4957(4)	6844(4)	1140(2)	27(1)
C(22)	5379(5)	6806(4)	145(2)	31(1)
C(23)	4500(4)	7019(4)	553(2)	29(1)
C(24)	3959(5)	6218(5)	569(2)	37(1)
C(25)	9207(4)	10458(4)	3304(2)	28(1)
C(26)	7825(4)	9283(5)	2096(2)	30(1)
C(27)	5191(4)	9440(4)	1891(2)	28(1)
C(28)	9985(4)	10815(4)	5526(2)	21(1)
C(29)	10464(4)	11729(4)	6147(2)	23(1)
C(30)	9808(4)	13014(4)	5939(2)	23(1)
C(31)	10366(4)	13846(4)	6596(2)	19(1)
C(32)	11430(4)	13603(4)	6378(2)	24(1)

C(33)	12167(4)	13883(4)	6598(2)	23(1)
C(34)	11859(4)	14431(4)	7029(2)	19(1)
C(35)	10824(4)	14676(4)	7257(2)	24(1)
C(36)	10099(4)	14382(4)	7047(2)	26(1)
C(37)	6314(4)	5363(4)	4330(2)	22(1)
C(38)	6406(4)	5822(4)	3722(2)	26(1)
C(39)	5592(4)	5669(4)	3372(2)	26(1)
C(40)	5791(4)	4426(4)	3457(2)	21(1)
C(41)	5800(4)	3935(4)	4089(2)	19(1)
C(42)	6510(4)	4145(4)	4461(2)	22(1)
C(43)	4830(4)	4387(4)	3150(2)	22(1)
C(44)	4804(4)	3232(4)	3352(2)	22(1)
C(45)	4552(4)	3035(4)	3972(2)	25(1)
C(46)	5216(4)	3359(4)	4305(2)	24(1)
C(47)	4826(4)	4764(4)	2510(2)	25(1)
C(48)	3952(4)	4621(4)	2196(2)	27(1)
C(49)	4076(4)	3418(4)	2364(2)	22(1)
C(50)	3949(4)	3145(4)	3001(2)	22(1)
C(51)	3821(4)	2055(4)	3133(2)	24(1)
C(52)	3178(4)	2138(4)	2614(2)	25(1)
C(53)	3125(4)	3185(4)	2162(2)	25(1)
C(54)	3132(4)	3029(4)	1562(2)	24(1)
C(55)	2117(4)	2855(5)	1425(2)	28(1)
C(56)	2253(4)	2358(4)	917(2)	27(1)
C(57)	1196(4)	2372(4)	703(2)	26(1)
C(58)	1321(4)	1949(5)	171(2)	32(1)
C(59)	159(5)	2205(6)	-66(3)	51(2)
C(60)	2106(5)	706(5)	251(3)	46(2)
C(61)	3183(4)	4016(4)	1125(2)	30(1)
C(62)	5233(4)	2570(4)	2202(2)	25(1)
C(63)	6957(4)	3743(4)	3239(2)	28(1)
C(64)	6864(4)	5706(4)	5147(2)	17(1)
C(65)	7477(4)	6289(4)	5882(2)	21(1)
C(66)	6777(4)	7572(4)	5716(2)	22(1)
C(67)	7348(4)	8423(4)	6358(2)	19(1)
C(68)	7047(4)	9099(4)	6750(2)	20(1)
C(69)	7780(4)	9432(4)	6932(2)	23(1)

C(70)	8846(4)	9074(4)	6729(2)	25(1)
C(71)	9174(4)	8415(4)	6335(2)	27(1)
C(72)	8445(4)	8076(4)	6154(2)	24(1)
C(73)	7008(4)	5681(4)	7609(2)	22(1)
C(74)	7644(4)	4847(4)	8138(2)	24(1)
C(75)	8293(4)	5270(4)	8427(2)	21(1)
C(76)	7644(4)	6474(4)	8510(2)	22(1)
C(77)	7072(4)	7247(4)	7948(2)	25(1)
C(78)	6323(4)	6862(4)	7686(2)	24(1)
C(79)	9383(4)	4626(4)	8582(2)	29(1)
C(80)	10060(4)	4939(4)	8910(2)	31(1)
C(81)	9300(4)	5933(4)	9167(2)	26(1)
C(82)	8455(4)	6879(4)	8716(2)	24(1)
C(83)	7854(5)	8015(4)	8880(2)	32(1)
C(84)	8584(4)	8356(4)	9183(2)	29(1)
C(85)	9244(4)	7405(4)	9688(2)	26(1)
C(86)	9978(4)	6363(4)	9445(2)	26(1)
C(87)	10809(5)	5504(4)	9922(2)	36(1)
C(88)	11003(4)	6274(4)	10245(2)	28(1)
C(89)	10156(4)	7529(4)	9993(2)	24(1)
C(90)	9815(4)	8245(4)	10430(2)	30(1)
C(91)	10858(4)	8173(5)	10711(2)	31(1)
C(92)	10646(4)	8696(5)	11215(2)	34(1)
C(93)	11695(5)	8246(5)	11589(2)	37(1)
C(94)	11529(5)	8689(5)	12126(2)	35(1)
C(95)	11287(6)	9921(5)	12010(3)	54(2)
C(96)	12532(6)	7969(6)	12542(3)	66(2)
C(97)	8984(5)	9485(5)	10196(2)	40(1)
C(98)	8429(4)	7178(5)	10123(2)	34(1)
C(99)	6742(4)	6488(4)	8942(2)	28(1)
C(100)	6721(4)	4413(4)	7181(2)	24(1)
C(101)	6351(4)	3022(4)	6877(2)	26(1)
C(102)	6545(4)	3263(4)	6250(2)	27(1)
C(103)	6069(4)	1999(4)	5846(2)	20(1)
C(104)	4917(4)	2610(4)	5906(2)	27(1)
C(105)	4162(4)	2319(4)	5716(2)	26(1)
C(106)	4526(4)	1407(4)	5478(2)	22(1)

C(107)	5661(4)	777(4)	5401(2)	22(1)
C(108)	6429(4)	1080(4)	5583(2)	22(1)
C(109)	3787(4)	9962(4)	7567(2)	22(1)
C(110)	3740(4)	11130(4)	7336(2)	28(1)
C(111)	4391(4)	11359(5)	7747(2)	28(1)
C(112)	3994(4)	11285(4)	8347(2)	22(1)
C(113)	3907(4)	10164(4)	8551(2)	20(1)
C(114)	3329(4)	9866(4)	8146(2)	23(1)
C(115)	4283(4)	9482(4)	9052(2)	25(1)
C(116)	4823(4)	9706(4)	9496(2)	24(1)
C(117)	4651(4)	10950(4)	9363(2)	21(1)
C(118)	4853(4)	11308(4)	8737(2)	22(1)
C(119)	4935(4)	12456(4)	8594(2)	29(1)
C(120)	5716(4)	12512(4)	9010(2)	27(1)
C(121)	5412(4)	12250(4)	9618(2)	23(1)
C(122)	5458(4)	11056(4)	9731(2)	22(1)
C(123)	5385(4)	10708(4)	10364(2)	26(1)
C(124)	6019(4)	11257(4)	10594(2)	25(1)
C(125)	6275(4)	12038(4)	10079(2)	21(1)
C(126)	6360(4)	13035(4)	10234(2)	29(1)
C(127)	7252(4)	12583(4)	10721(2)	29(1)
C(128)	7300(5)	13496(5)	10969(2)	31(1)
C(129)	8183(4)	12992(4)	11456(2)	29(1)
C(130)	8270(4)	13858(5)	11730(2)	29(1)
C(131)	9153(4)	13256(5)	12213(2)	34(1)
C(132)	8481(5)	14773(5)	11313(2)	35(1)
C(133)	6624(5)	13768(5)	9733(2)	35(1)
C(134)	4258(4)	13153(4)	9717(2)	28(1)
C(135)	2802(4)	12266(4)	8364(2)	31(1)
C(136)	3510(4)	9329(4)	6783(2)	18(1)
C(137)	3124(4)	8454(4)	6113(2)	24(1)
C(138)	3744(4)	7180(4)	6370(2)	24(1)
C(139)	3203(4)	6276(4)	5748(2)	20(1)
C(140)	3497(4)	5659(4)	5328(2)	21(1)
C(141)	2754(4)	5362(4)	5127(2)	25(1)
C(142)	1694(4)	5693(4)	5329(2)	28(1)
C(143)	1368(4)	6334(4)	5735(2)	29(1)

C(144)	2108(4)	6622(4)	5944(2)	23(1)
C(145)	2802(6)	6459(6)	8398(3)	51(2)
C(146)	9858(5)	836(5)	8223(2)	40(1)
C(147)	4065(5)	9101(5)	4160(2)	38(1)
C(148)	10905(4)	3114(5)	4149(3)	40(1)
N(1)	10709(3)	11155(3)	5689(2)	24(1)
N(2)	9614(3)	13590(3)	6387(2)	22(1)
N(3)	12635(4)	14730(3)	7249(2)	29(1)
N(4)	7688(3)	5817(3)	5388(2)	22(1)
N(5)	6607(3)	8111(3)	6179(2)	23(1)
N(6)	9630(4)	9417(4)	6907(2)	35(1)
N(7)	5985(3)	4028(3)	7092(2)	28(1)
N(8)	6846(3)	2282(3)	6013(2)	26(1)
N(9)	3727(4)	1063(4)	5309(2)	33(1)
N(10)	2795(3)	9084(3)	6548(2)	23(1)
N(11)	3972(3)	6512(3)	5955(2)	22(1)
N(12)	913(4)	5367(4)	5129(2)	35(1)
O(1)	10421(3)	10288(3)	5100(1)	24(1)
O(2)	9092(3)	10938(3)	5724(1)	26(1)
O(3)	13573(3)	14473(3)	7050(2)	35(1)
O(4)	12346(3)	15219(4)	7640(2)	46(1)
O(5)	7148(2)	5468(3)	4649(1)	22(1)
O(6)	5988(2)	5820(3)	5362(1)	23(1)
O(7)	9316(4)	10075(4)	7218(2)	48(1)
O(8)	10590(3)	9036(3)	6741(2)	41(1)
O(9)	6235(3)	5328(3)	7403(1)	26(1)
O(10)	7710(3)	3986(3)	7070(1)	28(1)
O(11)	2714(3)	1623(4)	5386(2)	50(1)
O(12)	4058(3)	259(3)	5095(2)	45(1)
O(13)	3058(3)	9782(3)	7222(1)	25(1)
O(14)	4451(3)	9168(3)	6628(1)	25(1)
O(15)	-63(3)	5775(3)	5280(2)	43(1)
O(16)	1251(3)	4683(4)	4834(2)	48(1)
Cl(1)	1818(2)	7705(2)	7961(1)	81(1)
Cl(2)	4104(2)	6020(2)	8105(1)	83(1)
Cl(3)	2892(2)	6697(2)	9062(1)	70(1)
Cl(4)	10172(1)	1887(1)	7807(1)	55(1)

Cl(5)	10702(2)	191(2)	8847(1)	64(1)
Cl(6)	8433(2)	1384(2)	8365(1)	80(1)
Cl(7)	3598(1)	8175(2)	4597(1)	69(1)
Cl(8)	5525(1)	8564(2)	4290(1)	51(1)
Cl(9)	3768(2)	9241(2)	3456(1)	58(1)
Cl(10)	9503(1)	3708(2)	4338(1)	55(1)
Cl(11)	11324(2)	1764(1)	4037(1)	67(1)
Cl(12)	11143(2)	4001(2)	3592(1)	81(1)

Table 3. Bond lengths [Å] and angles [°] for **1·Ch**.

C(1)-O(1)	1.473(5)
C(1)-C(6)	1.504(7)
C(1)-C(2)	1.505(7)
C(1)-H(1)	1.0000
C(2)-C(3)	1.521(6)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.554(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.514(7)
C(4)-C(25)	1.540(7)
C(4)-C(10)	1.542(7)
C(5)-C(7)	1.325(7)
C(5)-C(6)	1.507(7)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.495(8)
C(7)-H(7)	0.9500
C(8)-C(9)	1.539(7)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(14)	1.516(7)
C(9)-C(10)	1.537(7)
C(9)-H(9)	1.0000
C(10)-C(11)	1.557(7)
C(10)-H(10)	1.0000
C(11)-C(12)	1.509(7)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.533(7)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(26)	1.515(7)
C(13)-C(17)	1.543(7)

C(13)-C(14)	1.543(6)
C(14)-C(15)	1.533(8)
C(14)-H(14)	1.0000
C(15)-C(16)	1.540(8)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.561(8)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.541(6)
C(17)-H(17)	1.0000
C(18)-C(27)	1.531(7)
C(18)-C(19)	1.539(7)
C(18)-H(18)	1.0000
C(19)-C(20)	1.514(7)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-C(21)	1.522(7)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(23)	1.524(7)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.462(7)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.532(7)
C(23)-H(23)	1.0000
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-O(2)	1.208(5)
C(28)-N(1)	1.348(5)
C(28)-O(1)	1.361(5)
C(29)-N(1)	1.454(4)
C(29)-C(30)	1.526(7)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-N(2)	1.440(4)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-N(2)	1.354(5)
C(31)-C(32)	1.402(6)
C(31)-C(36)	1.407(6)
C(32)-C(33)	1.372(7)
C(32)-H(32)	0.9500
C(33)-C(34)	1.374(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.378(7)
C(34)-N(3)	1.433(5)
C(35)-C(36)	1.359(7)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(37)-O(5)	1.468(5)
C(37)-C(38)	1.493(7)
C(37)-C(42)	1.502(7)
C(37)-H(37)	1.0000
C(38)-C(39)	1.531(7)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.543(7)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(41)	1.532(6)

C(40)-C(43)	1.547(6)
C(40)-C(63)	1.549(6)
C(41)-C(46)	1.330(7)
C(41)-C(42)	1.507(6)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(47)	1.532(6)
C(43)-C(44)	1.534(7)
C(43)-H(43)	1.0000
C(44)-C(45)	1.523(6)
C(44)-C(50)	1.527(6)
C(44)-H(44)	1.0000
C(45)-C(46)	1.496(7)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-H(46)	0.9500
C(47)-C(48)	1.536(6)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.513(7)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.534(6)
C(49)-C(62)	1.553(7)
C(49)-C(53)	1.563(7)
C(50)-C(51)	1.513(7)
C(50)-H(50)	1.0000
C(51)-C(52)	1.532(6)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-C(53)	1.552(7)
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.536(7)
C(53)-H(53)	1.0000
C(54)-C(61)	1.522(7)
C(54)-C(55)	1.534(7)

C(54)-H(54)	1.0000
C(55)-C(56)	1.518(6)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-C(57)	1.517(6)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.520(7)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-C(60)	1.505(8)
C(58)-C(59)	1.542(7)
C(58)-H(58)	1.0000
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-H(63A)	0.9800
C(63)-H(63B)	0.9800
C(63)-H(63C)	0.9800
C(64)-O(6)	1.205(5)
C(64)-O(5)	1.328(4)
C(64)-N(4)	1.356(4)
C(65)-N(4)	1.457(4)
C(65)-C(66)	1.522(7)
C(65)-H(65A)	0.9900
C(65)-H(65B)	0.9900
C(66)-N(5)	1.447(4)
C(66)-H(66A)	0.9900

C(66)-H(66B)	0.9900
C(67)-N(5)	1.358(5)
C(67)-C(68)	1.404(6)
C(67)-C(72)	1.415(7)
C(68)-C(69)	1.372(7)
C(68)-H(68)	0.9500
C(69)-C(70)	1.379(7)
C(69)-H(69)	0.9500
C(70)-C(71)	1.392(7)
C(70)-N(6)	1.437(5)
C(71)-C(72)	1.372(7)
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
C(73)-O(9)	1.465(5)
C(73)-C(78)	1.499(7)
C(73)-C(74)	1.506(7)
C(73)-H(73)	1.0000
C(74)-C(75)	1.508(7)
C(74)-H(74A)	0.9900
C(74)-H(74B)	0.9900
C(75)-C(79)	1.339(7)
C(75)-C(76)	1.526(7)
C(76)-C(77)	1.522(6)
C(76)-C(99)	1.544(7)
C(76)-C(82)	1.559(7)
C(77)-C(78)	1.538(7)
C(77)-H(77A)	0.9900
C(77)-H(77B)	0.9900
C(78)-H(78A)	0.9900
C(78)-H(78B)	0.9900
C(79)-C(80)	1.491(7)
C(79)-H(79)	0.9500
C(80)-C(81)	1.532(7)
C(80)-H(80A)	0.9900
C(80)-H(80B)	0.9900
C(81)-C(82)	1.527(6)
C(81)-C(86)	1.530(7)

C(81)-H(81)	1.0000
C(82)-C(83)	1.525(7)
C(82)-H(82)	1.0000
C(83)-C(84)	1.535(7)
C(83)-H(83A)	0.9900
C(83)-H(83B)	0.9900
C(84)-C(85)	1.528(7)
C(84)-H(84A)	0.9900
C(84)-H(84B)	0.9900
C(85)-C(98)	1.546(7)
C(85)-C(89)	1.549(7)
C(85)-C(86)	1.550(7)
C(86)-C(87)	1.522(7)
C(86)-H(86)	1.0000
C(87)-C(88)	1.558(7)
C(87)-H(87A)	0.9900
C(87)-H(87B)	0.9900
C(88)-C(89)	1.556(7)
C(88)-H(88A)	0.9900
C(88)-H(88B)	0.9900
C(89)-C(90)	1.531(7)
C(89)-H(89)	1.0000
C(90)-C(97)	1.529(7)
C(90)-C(91)	1.539(7)
C(90)-H(90)	1.0000
C(91)-C(92)	1.519(7)
C(91)-H(91A)	0.9900
C(91)-H(91B)	0.9900
C(92)-C(93)	1.514(7)
C(92)-H(92A)	0.9900
C(92)-H(92B)	0.9900
C(93)-C(94)	1.540(7)
C(93)-H(93A)	0.9900
C(93)-H(93B)	0.9900
C(94)-C(95)	1.505(8)
C(94)-C(96)	1.521(8)
C(94)-H(94)	1.0000

C(95)-H(95A)	0.9800
C(95)-H(95B)	0.9800
C(95)-H(95C)	0.9800
C(96)-H(96A)	0.9800
C(96)-H(96B)	0.9800
C(96)-H(96C)	0.9800
C(97)-H(97A)	0.9800
C(97)-H(97B)	0.9800
C(97)-H(97C)	0.9800
C(98)-H(98A)	0.9800
C(98)-H(98B)	0.9800
C(98)-H(98C)	0.9800
C(99)-H(99A)	0.9800
C(99)-H(99B)	0.9800
C(99)-H(99C)	0.9800
C(100)-O(10)	1.220(5)
C(100)-N(7)	1.343(5)
C(100)-O(9)	1.347(5)
C(101)-N(7)	1.445(5)
C(101)-C(102)	1.525(7)
C(101)-H(10A)	0.9900
C(101)-H(10B)	0.9900
C(102)-N(8)	1.457(5)
C(102)-H(10C)	0.9900
C(102)-H(10D)	0.9900
C(103)-N(8)	1.361(5)
C(103)-C(104)	1.397(6)
C(103)-C(108)	1.418(6)
C(104)-C(105)	1.368(7)
C(104)-H(104)	0.9500
C(105)-C(106)	1.371(6)
C(105)-H(105)	0.9500
C(106)-C(107)	1.391(7)
C(106)-N(9)	1.447(5)
C(107)-C(108)	1.385(7)
C(107)-H(107)	0.9500
C(108)-H(108)	0.9500

C(109)-O(13)	1.458(5)
C(109)-C(114)	1.510(6)
C(109)-C(110)	1.517(7)
C(109)-H(109)	1.0000
C(110)-C(111)	1.535(7)
C(110)-H(11C)	0.9900
C(110)-H(11D)	0.9900
C(111)-C(112)	1.529(6)
C(111)-H(11E)	0.9900
C(111)-H(11F)	0.9900
C(112)-C(113)	1.530(7)
C(112)-C(118)	1.549(7)
C(112)-C(135)	1.557(7)
C(113)-C(115)	1.320(6)
C(113)-C(114)	1.516(6)
C(114)-H(11G)	0.9900
C(114)-H(11H)	0.9900
C(115)-C(116)	1.496(7)
C(115)-H(115)	0.9500
C(116)-C(117)	1.547(7)
C(116)-H(11I)	0.9900
C(116)-H(11J)	0.9900
C(117)-C(122)	1.517(6)
C(117)-C(118)	1.541(6)
C(117)-H(117)	1.0000
C(118)-C(119)	1.557(7)
C(118)-H(118)	1.0000
C(119)-C(120)	1.539(7)
C(119)-H(11K)	0.9900
C(119)-H(11L)	0.9900
C(120)-C(121)	1.520(7)
C(120)-H(12C)	0.9900
C(120)-H(12D)	0.9900
C(121)-C(134)	1.528(7)
C(121)-C(122)	1.543(7)
C(121)-C(125)	1.547(6)
C(122)-C(123)	1.522(6)

C(122)-H(122)	1.0000
C(123)-C(124)	1.545(7)
C(123)-H(12E)	0.9900
C(123)-H(12F)	0.9900
C(124)-C(125)	1.565(7)
C(124)-H(12G)	0.9900
C(124)-H(12H)	0.9900
C(125)-C(126)	1.536(7)
C(125)-H(125)	1.0000
C(126)-C(133)	1.512(7)
C(126)-C(127)	1.548(7)
C(126)-H(126)	1.0000
C(127)-C(128)	1.527(7)
C(127)-H(12I)	0.9900
C(127)-H(12J)	0.9900
C(128)-C(129)	1.530(7)
C(128)-H(12K)	0.9900
C(128)-H(12L)	0.9900
C(129)-C(130)	1.530(7)
C(129)-H(12M)	0.9900
C(129)-H(12N)	0.9900
C(130)-C(131)	1.521(7)
C(130)-C(132)	1.523(7)
C(130)-H(130)	1.0000
C(131)-H(13A)	0.9800
C(131)-H(13B)	0.9800
C(131)-H(13C)	0.9800
C(132)-H(13D)	0.9800
C(132)-H(13E)	0.9800
C(132)-H(13F)	0.9800
C(133)-H(13G)	0.9800
C(133)-H(13H)	0.9800
C(133)-H(13I)	0.9800
C(134)-H(13J)	0.9800
C(134)-H(13K)	0.9800
C(134)-H(13L)	0.9800
C(135)-H(13M)	0.9800

C(135)-H(13N)	0.9800
C(135)-H(13O)	0.9800
C(136)-O(14)	1.221(4)
C(136)-N(10)	1.333(5)
C(136)-O(13)	1.342(4)
C(137)-N(10)	1.451(5)
C(137)-C(138)	1.527(7)
C(137)-H(13P)	0.9900
C(137)-H(13Q)	0.9900
C(138)-N(11)	1.451(5)
C(138)-H(13R)	0.9900
C(138)-H(13S)	0.9900
C(139)-N(11)	1.353(5)
C(139)-C(144)	1.407(6)
C(139)-C(140)	1.408(6)
C(140)-C(141)	1.372(7)
C(140)-H(140)	0.9500
C(141)-C(142)	1.373(7)
C(141)-H(141)	0.9500
C(142)-C(143)	1.399(7)
C(142)-N(12)	1.443(5)
C(143)-C(144)	1.369(7)
C(143)-H(143)	0.9500
C(144)-H(144)	0.9500
C(145)-Cl(2)	1.730(6)
C(145)-Cl(1)	1.748(7)
C(145)-Cl(3)	1.757(6)
C(145)-H(145)	1.0000
C(146)-Cl(4)	1.733(6)
C(146)-Cl(6)	1.745(6)
C(146)-Cl(5)	1.754(6)
C(146)-H(146)	1.0000
C(147)-Cl(9)	1.745(5)
C(147)-Cl(7)	1.749(6)
C(147)-Cl(8)	1.761(6)
C(147)-H(147)	1.0000
C(148)-Cl(12)	1.702(6)

C(148)-Cl(11)	1.742(6)
C(148)-Cl(10)	1.752(5)
C(148)-H(148)	1.0000
N(1)-H(1')	0.88(2)
N(2)-H(2')	0.86(4)
N(3)-O(3)	1.237(5)
N(3)-O(4)	1.240(5)
N(4)-H(4')	0.85(5)
N(5)-H(5')	0.87(4)
N(6)-O(8)	1.227(5)
N(6)-O(7)	1.227(5)
N(7)-H(7')	0.89(4)
N(8)-H(8')	0.86(4)
N(9)-O(12)	1.213(5)
N(9)-O(11)	1.244(5)
N(10)-H(10')	0.88(5)
N(11)-H(11')	0.88(4)
N(12)-O(16)	1.221(5)
N(12)-O(15)	1.235(5)
O(1)-C(1)-C(6)	104.3(4)
O(1)-C(1)-C(2)	111.4(4)
C(6)-C(1)-C(2)	111.2(4)
O(1)-C(1)-H(1)	110.0
C(6)-C(1)-H(1)	110.0
C(2)-C(1)-H(1)	110.0
C(1)-C(2)-C(3)	108.7(4)
C(1)-C(2)-H(2A)	109.9
C(3)-C(2)-H(2A)	109.9
C(1)-C(2)-H(2B)	109.9
C(3)-C(2)-H(2B)	109.9
H(2A)-C(2)-H(2B)	108.3
C(2)-C(3)-C(4)	113.9(4)
C(2)-C(3)-H(3A)	108.8
C(4)-C(3)-H(3A)	108.8
C(2)-C(3)-H(3B)	108.8
C(4)-C(3)-H(3B)	108.8

H(3A)-C(3)-H(3B)	107.7
C(5)-C(4)-C(25)	108.2(4)
C(5)-C(4)-C(10)	109.3(4)
C(25)-C(4)-C(10)	112.1(4)
C(5)-C(4)-C(3)	108.1(4)
C(25)-C(4)-C(3)	108.5(4)
C(10)-C(4)-C(3)	110.6(4)
C(7)-C(5)-C(6)	119.9(5)
C(7)-C(5)-C(4)	122.6(4)
C(6)-C(5)-C(4)	117.4(4)
C(1)-C(6)-C(5)	113.4(4)
C(1)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6A)	108.9
C(1)-C(6)-H(6B)	108.9
C(5)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
C(5)-C(7)-C(8)	125.3(5)
C(5)-C(7)-H(7)	117.4
C(8)-C(7)-H(7)	117.4
C(7)-C(8)-C(9)	112.6(5)
C(7)-C(8)-H(8A)	109.1
C(9)-C(8)-H(8A)	109.1
C(7)-C(8)-H(8B)	109.1
C(9)-C(8)-H(8B)	109.1
H(8A)-C(8)-H(8B)	107.8
C(14)-C(9)-C(10)	111.3(4)
C(14)-C(9)-C(8)	111.5(4)
C(10)-C(9)-C(8)	108.0(4)
C(14)-C(9)-H(9)	108.7
C(10)-C(9)-H(9)	108.7
C(8)-C(9)-H(9)	108.7
C(9)-C(10)-C(4)	112.1(4)
C(9)-C(10)-C(11)	111.9(4)
C(4)-C(10)-C(11)	112.8(4)
C(9)-C(10)-H(10)	106.5
C(4)-C(10)-H(10)	106.5
C(11)-C(10)-H(10)	106.5

C(12)-C(11)-C(10)	114.2(4)
C(12)-C(11)-H(11A)	108.7
C(10)-C(11)-H(11A)	108.7
C(12)-C(11)-H(11B)	108.7
C(10)-C(11)-H(11B)	108.7
H(11A)-C(11)-H(11B)	107.6
C(11)-C(12)-C(13)	112.0(4)
C(11)-C(12)-H(12A)	109.2
C(13)-C(12)-H(12A)	109.2
C(11)-C(12)-H(12B)	109.2
C(13)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
C(26)-C(13)-C(12)	111.0(4)
C(26)-C(13)-C(17)	110.5(4)
C(12)-C(13)-C(17)	116.2(4)
C(26)-C(13)-C(14)	112.4(4)
C(12)-C(13)-C(14)	106.2(4)
C(17)-C(13)-C(14)	100.1(4)
C(9)-C(14)-C(15)	118.5(5)
C(9)-C(14)-C(13)	114.5(4)
C(15)-C(14)-C(13)	103.9(4)
C(9)-C(14)-H(14)	106.4
C(15)-C(14)-H(14)	106.4
C(13)-C(14)-H(14)	106.4
C(14)-C(15)-C(16)	103.1(5)
C(14)-C(15)-H(15A)	111.1
C(16)-C(15)-H(15A)	111.1
C(14)-C(15)-H(15B)	111.1
C(16)-C(15)-H(15B)	111.1
H(15A)-C(15)-H(15B)	109.1
C(15)-C(16)-C(17)	107.2(4)
C(15)-C(16)-H(16A)	110.3
C(17)-C(16)-H(16A)	110.3
C(15)-C(16)-H(16B)	110.3
C(17)-C(16)-H(16B)	110.3
H(16A)-C(16)-H(16B)	108.5
C(18)-C(17)-C(13)	119.2(4)

C(18)-C(17)-C(16)	111.7(4)
C(13)-C(17)-C(16)	103.4(4)
C(18)-C(17)-H(17)	107.4
C(13)-C(17)-H(17)	107.4
C(16)-C(17)-H(17)	107.4
C(27)-C(18)-C(19)	108.9(4)
C(27)-C(18)-C(17)	113.5(4)
C(19)-C(18)-C(17)	110.2(4)
C(27)-C(18)-H(18)	108.0
C(19)-C(18)-H(18)	108.0
C(17)-C(18)-H(18)	108.0
C(20)-C(19)-C(18)	115.2(4)
C(20)-C(19)-H(19A)	108.5
C(18)-C(19)-H(19A)	108.5
C(20)-C(19)-H(19B)	108.5
C(18)-C(19)-H(19B)	108.5
H(19A)-C(19)-H(19B)	107.5
C(19)-C(20)-C(21)	112.8(4)
C(19)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20A)	109.0
C(19)-C(20)-H(20B)	109.0
C(21)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-C(23)	114.2(4)
C(20)-C(21)-H(21A)	108.7
C(23)-C(21)-H(21A)	108.7
C(20)-C(21)-H(21B)	108.7
C(23)-C(21)-H(21B)	108.7
H(21A)-C(21)-H(21B)	107.6
C(23)-C(22)-H(22A)	109.5
C(23)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(23)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(22)-C(23)-C(21)	112.2(4)
C(22)-C(23)-C(24)	109.0(4)

C(21)-C(23)-C(24)	109.4(4)
C(22)-C(23)-H(23)	108.7
C(21)-C(23)-H(23)	108.7
C(24)-C(23)-H(23)	108.7
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(4)-C(25)-H(25A)	109.5
C(4)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(4)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(13)-C(26)-H(26A)	109.5
C(13)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(13)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(18)-C(27)-H(27A)	109.5
C(18)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(18)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(2)-C(28)-N(1)	126.5(4)
O(2)-C(28)-O(1)	124.1(4)
N(1)-C(28)-O(1)	109.4(3)
N(1)-C(29)-C(30)	112.0(3)
N(1)-C(29)-H(29A)	109.2
C(30)-C(29)-H(29A)	109.2
N(1)-C(29)-H(29B)	109.2
C(30)-C(29)-H(29B)	109.2
H(29A)-C(29)-H(29B)	107.9

N(2)-C(30)-C(29)	112.1(3)
N(2)-C(30)-H(30A)	109.2
C(29)-C(30)-H(30A)	109.2
N(2)-C(30)-H(30B)	109.2
C(29)-C(30)-H(30B)	109.2
H(30A)-C(30)-H(30B)	107.9
N(2)-C(31)-C(32)	122.4(4)
N(2)-C(31)-C(36)	120.5(4)
C(32)-C(31)-C(36)	117.0(4)
C(33)-C(32)-C(31)	120.7(4)
C(33)-C(32)-H(32)	119.6
C(31)-C(32)-H(32)	119.6
C(32)-C(33)-C(34)	120.2(4)
C(32)-C(33)-H(33)	119.9
C(34)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	120.6(4)
C(33)-C(34)-N(3)	119.4(4)
C(35)-C(34)-N(3)	120.0(4)
C(36)-C(35)-C(34)	119.4(4)
C(36)-C(35)-H(35)	120.3
C(34)-C(35)-H(35)	120.3
C(35)-C(36)-C(31)	122.0(5)
C(35)-C(36)-H(36)	119.0
C(31)-C(36)-H(36)	119.0
O(5)-C(37)-C(38)	107.8(4)
O(5)-C(37)-C(42)	109.8(3)
C(38)-C(37)-C(42)	112.9(4)
O(5)-C(37)-H(37)	108.8
C(38)-C(37)-H(37)	108.8
C(42)-C(37)-H(37)	108.8
C(37)-C(38)-C(39)	109.4(4)
C(37)-C(38)-H(38A)	109.8
C(39)-C(38)-H(38A)	109.8
C(37)-C(38)-H(38B)	109.8
C(39)-C(38)-H(38B)	109.8
H(38A)-C(38)-H(38B)	108.2
C(38)-C(39)-C(40)	114.2(4)

C(38)-C(39)-H(39A)	108.7
C(40)-C(39)-H(39A)	108.7
C(38)-C(39)-H(39B)	108.7
C(40)-C(39)-H(39B)	108.7
H(39A)-C(39)-H(39B)	107.6
C(41)-C(40)-C(39)	107.8(4)
C(41)-C(40)-C(43)	109.7(4)
C(39)-C(40)-C(43)	109.8(4)
C(41)-C(40)-C(63)	108.8(4)
C(39)-C(40)-C(63)	108.8(4)
C(43)-C(40)-C(63)	111.9(4)
C(46)-C(41)-C(42)	121.0(4)
C(46)-C(41)-C(40)	122.8(4)
C(42)-C(41)-C(40)	116.2(4)
C(37)-C(42)-C(41)	113.0(4)
C(37)-C(42)-H(42A)	109.0
C(41)-C(42)-H(42A)	109.0
C(37)-C(42)-H(42B)	109.0
C(41)-C(42)-H(42B)	109.0
H(42A)-C(42)-H(42B)	107.8
C(47)-C(43)-C(44)	113.2(4)
C(47)-C(43)-C(40)	113.1(4)
C(44)-C(43)-C(40)	111.5(4)
C(47)-C(43)-H(43)	106.1
C(44)-C(43)-H(43)	106.1
C(40)-C(43)-H(43)	106.1
C(45)-C(44)-C(50)	110.9(4)
C(45)-C(44)-C(43)	110.0(4)
C(50)-C(44)-C(43)	111.4(4)
C(45)-C(44)-H(44)	108.2
C(50)-C(44)-H(44)	108.2
C(43)-C(44)-H(44)	108.2
C(46)-C(45)-C(44)	111.6(4)
C(46)-C(45)-H(45A)	109.3
C(44)-C(45)-H(45A)	109.3
C(46)-C(45)-H(45B)	109.3
C(44)-C(45)-H(45B)	109.3

H(45A)-C(45)-H(45B)	108.0
C(41)-C(46)-C(45)	125.3(4)
C(41)-C(46)-H(46)	117.4
C(45)-C(46)-H(46)	117.4
C(43)-C(47)-C(48)	113.9(4)
C(43)-C(47)-H(47A)	108.8
C(48)-C(47)-H(47A)	108.8
C(43)-C(47)-H(47B)	108.8
C(48)-C(47)-H(47B)	108.8
H(47A)-C(47)-H(47B)	107.7
C(49)-C(48)-C(47)	111.9(4)
C(49)-C(48)-H(48A)	109.2
C(47)-C(48)-H(48A)	109.2
C(49)-C(48)-H(48B)	109.2
C(47)-C(48)-H(48B)	109.2
H(48A)-C(48)-H(48B)	107.9
C(48)-C(49)-C(50)	107.0(4)
C(48)-C(49)-C(62)	111.0(4)
C(50)-C(49)-C(62)	111.1(4)
C(48)-C(49)-C(53)	117.9(4)
C(50)-C(49)-C(53)	99.9(4)
C(62)-C(49)-C(53)	109.3(4)
C(51)-C(50)-C(44)	118.8(4)
C(51)-C(50)-C(49)	105.4(4)
C(44)-C(50)-C(49)	115.0(4)
C(51)-C(50)-H(50)	105.5
C(44)-C(50)-H(50)	105.5
C(49)-C(50)-H(50)	105.5
C(50)-C(51)-C(52)	104.1(4)
C(50)-C(51)-H(51A)	110.9
C(52)-C(51)-H(51A)	110.9
C(50)-C(51)-H(51B)	110.9
C(52)-C(51)-H(51B)	110.9
H(51A)-C(51)-H(51B)	108.9
C(51)-C(52)-C(53)	107.2(4)
C(51)-C(52)-H(52A)	110.3
C(53)-C(52)-H(52A)	110.3

C(51)-C(52)-H(52B)	110.3
C(53)-C(52)-H(52B)	110.3
H(52A)-C(52)-H(52B)	108.5
C(54)-C(53)-C(52)	112.5(4)
C(54)-C(53)-C(49)	118.8(4)
C(52)-C(53)-C(49)	103.7(4)
C(54)-C(53)-H(53)	107.0
C(52)-C(53)-H(53)	107.0
C(49)-C(53)-H(53)	107.0
C(61)-C(54)-C(55)	110.1(4)
C(61)-C(54)-C(53)	111.9(4)
C(55)-C(54)-C(53)	112.0(4)
C(61)-C(54)-H(54)	107.5
C(55)-C(54)-H(54)	107.5
C(53)-C(54)-H(54)	107.5
C(56)-C(55)-C(54)	113.9(4)
C(56)-C(55)-H(55A)	108.8
C(54)-C(55)-H(55A)	108.8
C(56)-C(55)-H(55B)	108.8
C(54)-C(55)-H(55B)	108.8
H(55A)-C(55)-H(55B)	107.7
C(55)-C(56)-C(57)	115.4(4)
C(55)-C(56)-H(56A)	108.4
C(57)-C(56)-H(56A)	108.4
C(55)-C(56)-H(56B)	108.4
C(57)-C(56)-H(56B)	108.4
H(56A)-C(56)-H(56B)	107.5
C(56)-C(57)-C(58)	115.0(4)
C(56)-C(57)-H(57A)	108.5
C(58)-C(57)-H(57A)	108.5
C(56)-C(57)-H(57B)	108.5
C(58)-C(57)-H(57B)	108.5
H(57A)-C(57)-H(57B)	107.5
C(60)-C(58)-C(57)	113.3(5)
C(60)-C(58)-C(59)	110.3(5)
C(57)-C(58)-C(59)	110.4(4)
C(60)-C(58)-H(58)	107.5

C(57)-C(58)-H(58)	107.5
C(59)-C(58)-H(58)	107.5
C(58)-C(59)-H(59A)	109.5
C(58)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(58)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(58)-C(60)-H(60A)	109.5
C(58)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(58)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(54)-C(61)-H(61A)	109.5
C(54)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(54)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(49)-C(62)-H(62A)	109.5
C(49)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(49)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(40)-C(63)-H(63A)	109.5
C(40)-C(63)-H(63B)	109.5
H(63A)-C(63)-H(63B)	109.5
C(40)-C(63)-H(63C)	109.5
H(63A)-C(63)-H(63C)	109.5
H(63B)-C(63)-H(63C)	109.5
O(6)-C(64)-O(5)	125.3(4)
O(6)-C(64)-N(4)	123.5(3)
O(5)-C(64)-N(4)	111.2(3)
N(4)-C(65)-C(66)	110.3(3)
N(4)-C(65)-H(65A)	109.6

C(66)-C(65)-H(65A)	109.6
N(4)-C(65)-H(65B)	109.6
C(66)-C(65)-H(65B)	109.6
H(65A)-C(65)-H(65B)	108.1
N(5)-C(66)-C(65)	113.4(3)
N(5)-C(66)-H(66A)	108.9
C(65)-C(66)-H(66A)	108.9
N(5)-C(66)-H(66B)	108.9
C(65)-C(66)-H(66B)	108.9
H(66A)-C(66)-H(66B)	107.7
N(5)-C(67)-C(68)	120.9(4)
N(5)-C(67)-C(72)	121.1(4)
C(68)-C(67)-C(72)	118.1(4)
C(69)-C(68)-C(67)	121.8(4)
C(69)-C(68)-H(68)	119.1
C(67)-C(68)-H(68)	119.1
C(68)-C(69)-C(70)	118.8(4)
C(68)-C(69)-H(69)	120.6
C(70)-C(69)-H(69)	120.6
C(69)-C(70)-C(71)	121.2(5)
C(69)-C(70)-N(6)	120.2(4)
C(71)-C(70)-N(6)	118.5(4)
C(72)-C(71)-C(70)	120.0(4)
C(72)-C(71)-H(71)	120.0
C(70)-C(71)-H(71)	120.0
C(71)-C(72)-C(67)	120.0(4)
C(71)-C(72)-H(72)	120.0
C(67)-C(72)-H(72)	120.0
O(9)-C(73)-C(78)	107.3(3)
O(9)-C(73)-C(74)	110.5(4)
C(78)-C(73)-C(74)	113.3(4)
O(9)-C(73)-H(73)	108.5
C(78)-C(73)-H(73)	108.5
C(74)-C(73)-H(73)	108.5
C(73)-C(74)-C(75)	112.9(4)
C(73)-C(74)-H(74A)	109.0
C(75)-C(74)-H(74A)	109.0

C(73)-C(74)-H(74B)	109.0
C(75)-C(74)-H(74B)	109.0
H(74A)-C(74)-H(74B)	107.8
C(79)-C(75)-C(74)	121.1(4)
C(79)-C(75)-C(76)	122.8(4)
C(74)-C(75)-C(76)	116.1(4)
C(77)-C(76)-C(75)	107.7(4)
C(77)-C(76)-C(99)	109.4(4)
C(75)-C(76)-C(99)	108.6(4)
C(77)-C(76)-C(82)	109.8(4)
C(75)-C(76)-C(82)	110.7(4)
C(99)-C(76)-C(82)	110.6(4)
C(76)-C(77)-C(78)	113.8(4)
C(76)-C(77)-H(77A)	108.8
C(78)-C(77)-H(77A)	108.8
C(76)-C(77)-H(77B)	108.8
C(78)-C(77)-H(77B)	108.8
H(77A)-C(77)-H(77B)	107.7
C(73)-C(78)-C(77)	109.9(4)
C(73)-C(78)-H(78A)	109.7
C(77)-C(78)-H(78A)	109.7
C(73)-C(78)-H(78B)	109.7
C(77)-C(78)-H(78B)	109.7
H(78A)-C(78)-H(78B)	108.2
C(75)-C(79)-C(80)	124.4(5)
C(75)-C(79)-H(79)	117.8
C(80)-C(79)-H(79)	117.8
C(79)-C(80)-C(81)	111.1(4)
C(79)-C(80)-H(80A)	109.4
C(81)-C(80)-H(80A)	109.4
C(79)-C(80)-H(80B)	109.4
C(81)-C(80)-H(80B)	109.4
H(80A)-C(80)-H(80B)	108.0
C(82)-C(81)-C(86)	111.6(4)
C(82)-C(81)-C(80)	109.3(4)
C(86)-C(81)-C(80)	112.0(4)
C(82)-C(81)-H(81)	107.9

C(86)-C(81)-H(81)	107.9
C(80)-C(81)-H(81)	107.9
C(83)-C(82)-C(81)	113.8(4)
C(83)-C(82)-C(76)	113.9(4)
C(81)-C(82)-C(76)	110.4(4)
C(83)-C(82)-H(82)	106.0
C(81)-C(82)-H(82)	106.0
C(76)-C(82)-H(82)	106.0
C(82)-C(83)-C(84)	116.3(4)
C(82)-C(83)-H(83A)	108.2
C(84)-C(83)-H(83A)	108.2
C(82)-C(83)-H(83B)	108.2
C(84)-C(83)-H(83B)	108.2
H(83A)-C(83)-H(83B)	107.4
C(85)-C(84)-C(83)	110.8(4)
C(85)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84A)	109.5
C(85)-C(84)-H(84B)	109.5
C(83)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	108.1
C(84)-C(85)-C(98)	110.4(4)
C(84)-C(85)-C(89)	117.8(4)
C(98)-C(85)-C(89)	109.2(4)
C(84)-C(85)-C(86)	105.5(4)
C(98)-C(85)-C(86)	112.7(4)
C(89)-C(85)-C(86)	101.0(4)
C(87)-C(86)-C(81)	116.2(4)
C(87)-C(86)-C(85)	105.3(4)
C(81)-C(86)-C(85)	114.0(4)
C(87)-C(86)-H(86)	106.9
C(81)-C(86)-H(86)	106.9
C(85)-C(86)-H(86)	106.9
C(86)-C(87)-C(88)	102.8(4)
C(86)-C(87)-H(87A)	111.2
C(88)-C(87)-H(87A)	111.2
C(86)-C(87)-H(87B)	111.2
C(88)-C(87)-H(87B)	111.2

H(87A)-C(87)-H(87B)	109.1
C(89)-C(88)-C(87)	108.3(4)
C(89)-C(88)-H(88A)	110.0
C(87)-C(88)-H(88A)	110.0
C(89)-C(88)-H(88B)	110.0
C(87)-C(88)-H(88B)	110.0
H(88A)-C(88)-H(88B)	108.4
C(90)-C(89)-C(85)	119.8(4)
C(90)-C(89)-C(88)	112.1(4)
C(85)-C(89)-C(88)	102.9(4)
C(90)-C(89)-H(89)	107.1
C(85)-C(89)-H(89)	107.1
C(88)-C(89)-H(89)	107.1
C(97)-C(90)-C(89)	113.5(4)
C(97)-C(90)-C(91)	110.4(4)
C(89)-C(90)-C(91)	111.0(4)
C(97)-C(90)-H(90)	107.2
C(89)-C(90)-H(90)	107.2
C(91)-C(90)-H(90)	107.2
C(92)-C(91)-C(90)	116.0(4)
C(92)-C(91)-H(91A)	108.3
C(90)-C(91)-H(91A)	108.3
C(92)-C(91)-H(91B)	108.3
C(90)-C(91)-H(91B)	108.3
H(91A)-C(91)-H(91B)	107.4
C(93)-C(92)-C(91)	112.8(4)
C(93)-C(92)-H(92A)	109.0
C(91)-C(92)-H(92A)	109.0
C(93)-C(92)-H(92B)	109.0
C(91)-C(92)-H(92B)	109.0
H(92A)-C(92)-H(92B)	107.8
C(92)-C(93)-C(94)	115.7(4)
C(92)-C(93)-H(93A)	108.4
C(94)-C(93)-H(93A)	108.4
C(92)-C(93)-H(93B)	108.4
C(94)-C(93)-H(93B)	108.4
H(93A)-C(93)-H(93B)	107.4

C(95)-C(94)-C(96)	110.3(5)
C(95)-C(94)-C(93)	113.0(5)
C(96)-C(94)-C(93)	111.4(5)
C(95)-C(94)-H(94)	107.3
C(96)-C(94)-H(94)	107.3
C(93)-C(94)-H(94)	107.3
C(94)-C(95)-H(95A)	109.5
C(94)-C(95)-H(95B)	109.5
H(95A)-C(95)-H(95B)	109.5
C(94)-C(95)-H(95C)	109.5
H(95A)-C(95)-H(95C)	109.5
H(95B)-C(95)-H(95C)	109.5
C(94)-C(96)-H(96A)	109.5
C(94)-C(96)-H(96B)	109.5
H(96A)-C(96)-H(96B)	109.5
C(94)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5
H(96B)-C(96)-H(96C)	109.5
C(90)-C(97)-H(97A)	109.5
C(90)-C(97)-H(97B)	109.5
H(97A)-C(97)-H(97B)	109.5
C(90)-C(97)-H(97C)	109.5
H(97A)-C(97)-H(97C)	109.5
H(97B)-C(97)-H(97C)	109.5
C(85)-C(98)-H(98A)	109.5
C(85)-C(98)-H(98B)	109.5
H(98A)-C(98)-H(98B)	109.5
C(85)-C(98)-H(98C)	109.5
H(98A)-C(98)-H(98C)	109.5
H(98B)-C(98)-H(98C)	109.5
C(76)-C(99)-H(99A)	109.5
C(76)-C(99)-H(99B)	109.5
H(99A)-C(99)-H(99B)	109.5
C(76)-C(99)-H(99C)	109.5
H(99A)-C(99)-H(99C)	109.5
H(99B)-C(99)-H(99C)	109.5
O(10)-C(100)-N(7)	123.7(4)

O(10)-C(100)-O(9)	124.4(4)
N(7)-C(100)-O(9)	111.9(3)
N(7)-C(101)-C(102)	111.7(4)
N(7)-C(101)-H(10A)	109.3
C(102)-C(101)-H(10A)	109.3
N(7)-C(101)-H(10B)	109.3
C(102)-C(101)-H(10B)	109.3
H(10A)-C(101)-H(10B)	107.9
N(8)-C(102)-C(101)	113.0(4)
N(8)-C(102)-H(10C)	109.0
C(101)-C(102)-H(10C)	109.0
N(8)-C(102)-H(10D)	109.0
C(101)-C(102)-H(10D)	109.0
H(10C)-C(102)-H(10D)	107.8
N(8)-C(103)-C(104)	122.3(4)
N(8)-C(103)-C(108)	119.3(4)
C(104)-C(103)-C(108)	118.4(4)
C(105)-C(104)-C(103)	120.3(4)
C(105)-C(104)-H(104)	119.8
C(103)-C(104)-H(104)	119.8
C(104)-C(105)-C(106)	120.6(4)
C(104)-C(105)-H(105)	119.7
C(106)-C(105)-H(105)	119.7
C(105)-C(106)-C(107)	121.5(4)
C(105)-C(106)-N(9)	120.1(4)
C(107)-C(106)-N(9)	118.3(4)
C(108)-C(107)-C(106)	118.3(4)
C(108)-C(107)-H(107)	120.9
C(106)-C(107)-H(107)	120.9
C(107)-C(108)-C(103)	120.9(4)
C(107)-C(108)-H(108)	119.6
C(103)-C(108)-H(108)	119.6
O(13)-C(109)-C(114)	105.2(3)
O(13)-C(109)-C(110)	110.1(3)
C(114)-C(109)-C(110)	111.0(4)
O(13)-C(109)-H(109)	110.2
C(114)-C(109)-H(109)	110.2

C(110)-C(109)-H(109)	110.2
C(109)-C(110)-C(111)	109.1(4)
C(109)-C(110)-H(11C)	109.9
C(111)-C(110)-H(11C)	109.9
C(109)-C(110)-H(11D)	109.9
C(111)-C(110)-H(11D)	109.9
H(11C)-C(110)-H(11D)	108.3
C(112)-C(111)-C(110)	115.8(4)
C(112)-C(111)-H(11E)	108.3
C(110)-C(111)-H(11E)	108.3
C(112)-C(111)-H(11F)	108.3
C(110)-C(111)-H(11F)	108.3
H(11E)-C(111)-H(11F)	107.4
C(111)-C(112)-C(113)	108.2(4)
C(111)-C(112)-C(118)	110.1(4)
C(113)-C(112)-C(118)	109.2(4)
C(111)-C(112)-C(135)	110.7(4)
C(113)-C(112)-C(135)	107.6(4)
C(118)-C(112)-C(135)	111.0(4)
C(115)-C(113)-C(114)	120.1(4)
C(115)-C(113)-C(112)	123.5(4)
C(114)-C(113)-C(112)	116.4(4)
C(109)-C(114)-C(113)	112.6(4)
C(109)-C(114)-H(11G)	109.1
C(113)-C(114)-H(11G)	109.1
C(109)-C(114)-H(11H)	109.1
C(113)-C(114)-H(11H)	109.1
H(11G)-C(114)-H(11H)	107.8
C(113)-C(115)-C(116)	125.1(4)
C(113)-C(115)-H(115)	117.5
C(116)-C(115)-H(115)	117.5
C(115)-C(116)-C(117)	112.3(4)
C(115)-C(116)-H(11I)	109.2
C(117)-C(116)-H(11I)	109.2
C(115)-C(116)-H(11J)	109.2
C(117)-C(116)-H(11J)	109.2
H(11I)-C(116)-H(11J)	107.9

C(122)-C(117)-C(118)	110.7(4)
C(122)-C(117)-C(116)	110.0(4)
C(118)-C(117)-C(116)	108.7(4)
C(122)-C(117)-H(117)	109.2
C(118)-C(117)-H(117)	109.2
C(116)-C(117)-H(117)	109.2
C(117)-C(118)-C(112)	112.2(4)
C(117)-C(118)-C(119)	112.0(4)
C(112)-C(118)-C(119)	113.2(4)
C(117)-C(118)-H(118)	106.3
C(112)-C(118)-H(118)	106.3
C(119)-C(118)-H(118)	106.3
C(120)-C(119)-C(118)	113.1(4)
C(120)-C(119)-H(11K)	109.0
C(118)-C(119)-H(11K)	109.0
C(120)-C(119)-H(11L)	109.0
C(118)-C(119)-H(11L)	109.0
H(11K)-C(119)-H(11L)	107.8
C(121)-C(120)-C(119)	113.1(4)
C(121)-C(120)-H(12C)	109.0
C(119)-C(120)-H(12C)	109.0
C(121)-C(120)-H(12D)	109.0
C(119)-C(120)-H(12D)	109.0
H(12C)-C(120)-H(12D)	107.8
C(120)-C(121)-C(134)	111.0(4)
C(120)-C(121)-C(122)	105.8(4)
C(134)-C(121)-C(122)	112.7(4)
C(120)-C(121)-C(125)	117.4(4)
C(134)-C(121)-C(125)	109.6(4)
C(122)-C(121)-C(125)	99.8(4)
C(117)-C(122)-C(123)	117.2(4)
C(117)-C(122)-C(121)	115.0(4)
C(123)-C(122)-C(121)	105.1(3)
C(117)-C(122)-H(122)	106.2
C(123)-C(122)-H(122)	106.2
C(121)-C(122)-H(122)	106.2
C(122)-C(123)-C(124)	103.1(4)

C(122)-C(123)-H(12E)	111.1
C(124)-C(123)-H(12E)	111.1
C(122)-C(123)-H(12F)	111.1
C(124)-C(123)-H(12F)	111.1
H(12E)-C(123)-H(12F)	109.1
C(123)-C(124)-C(125)	107.3(4)
C(123)-C(124)-H(12G)	110.3
C(125)-C(124)-H(12G)	110.3
C(123)-C(124)-H(12H)	110.3
C(125)-C(124)-H(12H)	110.3
H(12G)-C(124)-H(12H)	108.5
C(126)-C(125)-C(121)	120.8(4)
C(126)-C(125)-C(124)	112.5(4)
C(121)-C(125)-C(124)	103.2(4)
C(126)-C(125)-H(125)	106.5
C(121)-C(125)-H(125)	106.5
C(124)-C(125)-H(125)	106.5
C(133)-C(126)-C(125)	111.6(4)
C(133)-C(126)-C(127)	111.0(4)
C(125)-C(126)-C(127)	109.9(4)
C(133)-C(126)-H(126)	108.1
C(125)-C(126)-H(126)	108.1
C(127)-C(126)-H(126)	108.1
C(128)-C(127)-C(126)	114.8(4)
C(128)-C(127)-H(12I)	108.6
C(126)-C(127)-H(12I)	108.6
C(128)-C(127)-H(12J)	108.6
C(126)-C(127)-H(12J)	108.6
H(12I)-C(127)-H(12J)	107.5
C(127)-C(128)-C(129)	112.2(4)
C(127)-C(128)-H(12K)	109.2
C(129)-C(128)-H(12K)	109.2
C(127)-C(128)-H(12L)	109.2
C(129)-C(128)-H(12L)	109.2
H(12K)-C(128)-H(12L)	107.9
C(130)-C(129)-C(128)	115.2(4)
C(130)-C(129)-H(12M)	108.5

C(128)-C(129)-H(12M)	108.5
C(130)-C(129)-H(12N)	108.5
C(128)-C(129)-H(12N)	108.5
H(12M)-C(129)-H(12N)	107.5
C(131)-C(130)-C(132)	111.7(5)
C(131)-C(130)-C(129)	110.3(4)
C(132)-C(130)-C(129)	113.1(4)
C(131)-C(130)-H(130)	107.1
C(132)-C(130)-H(130)	107.1
C(129)-C(130)-H(130)	107.1
C(130)-C(131)-H(13A)	109.5
C(130)-C(131)-H(13B)	109.5
H(13A)-C(131)-H(13B)	109.5
C(130)-C(131)-H(13C)	109.5
H(13A)-C(131)-H(13C)	109.5
H(13B)-C(131)-H(13C)	109.5
C(130)-C(132)-H(13D)	109.5
C(130)-C(132)-H(13E)	109.5
H(13D)-C(132)-H(13E)	109.5
C(130)-C(132)-H(13F)	109.5
H(13D)-C(132)-H(13F)	109.5
H(13E)-C(132)-H(13F)	109.5
C(126)-C(133)-H(13G)	109.5
C(126)-C(133)-H(13H)	109.5
H(13G)-C(133)-H(13H)	109.5
C(126)-C(133)-H(13I)	109.5
H(13G)-C(133)-H(13I)	109.5
H(13H)-C(133)-H(13I)	109.5
C(121)-C(134)-H(13J)	109.5
C(121)-C(134)-H(13K)	109.5
H(13J)-C(134)-H(13K)	109.5
C(121)-C(134)-H(13L)	109.5
H(13J)-C(134)-H(13L)	109.5
H(13K)-C(134)-H(13L)	109.5
C(112)-C(135)-H(13M)	109.5
C(112)-C(135)-H(13N)	109.5
H(13M)-C(135)-H(13N)	109.5

C(112)-C(135)-H(13O)	109.5
H(13M)-C(135)-H(13O)	109.5
H(13N)-C(135)-H(13O)	109.5
O(14)-C(136)-N(10)	125.6(3)
O(14)-C(136)-O(13)	123.6(4)
N(10)-C(136)-O(13)	110.8(3)
N(10)-C(137)-C(138)	110.6(3)
N(10)-C(137)-H(13P)	109.5
C(138)-C(137)-H(13P)	109.5
N(10)-C(137)-H(13Q)	109.5
C(138)-C(137)-H(13Q)	109.5
H(13P)-C(137)-H(13Q)	108.1
N(11)-C(138)-C(137)	112.4(4)
N(11)-C(138)-H(13R)	109.1
C(137)-C(138)-H(13R)	109.1
N(11)-C(138)-H(13S)	109.1
C(137)-C(138)-H(13S)	109.1
H(13R)-C(138)-H(13S)	107.9
N(11)-C(139)-C(144)	121.8(4)
N(11)-C(139)-C(140)	119.8(4)
C(144)-C(139)-C(140)	118.4(4)
C(141)-C(140)-C(139)	121.2(4)
C(141)-C(140)-H(140)	119.4
C(139)-C(140)-H(140)	119.4
C(140)-C(141)-C(142)	119.5(5)
C(140)-C(141)-H(141)	120.2
C(142)-C(141)-H(141)	120.2
C(141)-C(142)-C(143)	120.5(5)
C(141)-C(142)-N(12)	120.0(4)
C(143)-C(142)-N(12)	119.6(4)
C(144)-C(143)-C(142)	120.5(5)
C(144)-C(143)-H(143)	119.8
C(142)-C(143)-H(143)	119.8
C(143)-C(144)-C(139)	119.8(4)
C(143)-C(144)-H(144)	120.1
C(139)-C(144)-H(144)	120.1
Cl(2)-C(145)-Cl(1)	110.3(3)

Cl(2)-C(145)-Cl(3)	110.3(4)
Cl(1)-C(145)-Cl(3)	109.6(3)
Cl(2)-C(145)-H(145)	108.9
Cl(1)-C(145)-H(145)	108.9
Cl(3)-C(145)-H(145)	108.9
Cl(4)-C(146)-Cl(6)	110.8(3)
Cl(4)-C(146)-Cl(5)	111.1(3)
Cl(6)-C(146)-Cl(5)	110.9(3)
Cl(4)-C(146)-H(146)	108.0
Cl(6)-C(146)-H(146)	108.0
Cl(5)-C(146)-H(146)	108.0
Cl(9)-C(147)-Cl(7)	110.6(3)
Cl(9)-C(147)-Cl(8)	110.4(3)
Cl(7)-C(147)-Cl(8)	108.6(3)
Cl(9)-C(147)-H(147)	109.1
Cl(7)-C(147)-H(147)	109.1
Cl(8)-C(147)-H(147)	109.1
Cl(12)-C(148)-Cl(11)	112.4(3)
Cl(12)-C(148)-Cl(10)	111.5(3)
Cl(11)-C(148)-Cl(10)	111.8(3)
Cl(12)-C(148)-H(148)	106.9
Cl(11)-C(148)-H(148)	106.9
Cl(10)-C(148)-H(148)	106.9
C(28)-N(1)-C(29)	121.2(3)
C(28)-N(1)-H(1')	119(3)
C(29)-N(1)-H(1')	118(3)
C(31)-N(2)-C(30)	125.3(3)
C(31)-N(2)-H(2')	107(3)
C(30)-N(2)-H(2')	124(3)
O(3)-N(3)-O(4)	122.4(4)
O(3)-N(3)-C(34)	119.0(4)
O(4)-N(3)-C(34)	118.6(4)
C(64)-N(4)-C(65)	120.6(3)
C(64)-N(4)-H(4')	114(3)
C(65)-N(4)-H(4')	125(3)
C(67)-N(5)-C(66)	124.5(3)
C(67)-N(5)-H(5')	116(3)

C(66)-N(5)-H(5')	116(3)
O(8)-N(6)-O(7)	122.6(4)
O(8)-N(6)-C(70)	118.5(4)
O(7)-N(6)-C(70)	118.9(4)
C(100)-N(7)-C(101)	120.5(3)
C(100)-N(7)-H(7')	122(3)
C(101)-N(7)-H(7')	117(3)
C(103)-N(8)-C(102)	123.0(3)
C(103)-N(8)-H(8')	116(3)
C(102)-N(8)-H(8')	121(3)
O(12)-N(9)-O(11)	122.6(4)
O(12)-N(9)-C(106)	119.5(4)
O(11)-N(9)-C(106)	117.9(4)
C(136)-N(10)-C(137)	122.0(3)
C(136)-N(10)-H(10')	114(3)
C(137)-N(10)-H(10')	120(3)
C(139)-N(11)-C(138)	124.3(3)
C(139)-N(11)-H(11')	112(3)
C(138)-N(11)-H(11')	123(3)
O(16)-N(12)-O(15)	123.3(4)
O(16)-N(12)-C(142)	119.0(4)
O(15)-N(12)-C(142)	117.7(4)
C(28)-O(1)-C(1)	118.4(3)
C(64)-O(5)-C(37)	117.1(3)
C(100)-O(9)-C(73)	115.7(3)
C(136)-O(13)-C(109)	117.4(3)

Symmetry transformations used to generate equivalent atoms:

