Synthesis of α-Amino Acids via Asymmetric Phase Transfer-Catalyzed Alkylation of Achiral Nickel(II) Complexes of Glycine-Derived Schiff Bases

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Contents

X-ray data and ORTEP diagrams for **1**, **2**, **32b**, **32d**, and **32f**.

The X-ray data for **1** and **2** were obtained at 110 K using Oxford Cryostream low-temperature device on a Smart 1000KappaCCD diffractometer with Mo K_α radiation (λ = 0.71069 Å), a graphite monochromator, and the φ and ω scan mode. Data reduction was performed with Saint PLUS v. 6.01 Bruker (1998) SAINTPlus Data Reduction and Correction Program v. 6.01, Bruker AXS, Madison, Wisconsin, USA. The absorption correction was applied semi-empirically using the SADABS program (Sheldrick G. M. (1998) SADABS v.2.01, Bruker/Siemens Area Detector Absorption Correction Program, Bruker AXS, Madison, Wisconsin, USA). Structures were solved by direct methods and refined by full matrix least-square (Sheldrick G. M. (1998) SHELXTL v.5.10, Structure Determination Software Suite, Bruker AXS, Madison, Wisconsin, USA).

Crystal data for **1**: $C_{21}H_{15}N_3NiO_3$, M = 416.07. Crystals were obtained from $CHCl_3$ at 110 K; they are monoclinic, space group $P2_1/c$, a = 12.783(3) Å, b = 8.550(4) Å, c = 7.234(1) Å, β = 101.687(5)°, V = 1679.8(6) $Å^3$, Z = 4, d_{calc} = 1.645 g cm^{-3}, μ =11.85 mm^{-1}. A total of 9250 reflections were measured, 3982 of them unique (R_{int} = 0.0362), with 2581 having I > 2σ(I). All 3982 reflections were used in the structure refinement based on F^2 by full-matrix least-squares techniques. Hydrogen atoms were located from Fourrier electron density synthesis and included into refinement in isotropic approximation. Final R_F = 0.0528 for observed data and wR2 = 0.1228 on F^2 for all data.

Crystal data for **2**: $C_{22}H_{17}N_3NiO_3$, M = 430.10. Crystals were obtained from $CHCl_3$ at 110K they are monoclinic, space group $P2_1/n$, a = 7.987(4)Å, b = 21.557(10)Å, c = 10.936(5)Å, β = 110.403(9)º, V = 1764.9(14) $Å^3$, Z = 4, d_{cal} = 1.619 g cm^{-3}, μ = 11.31 mm^{-1}. A total of 10376 reflections were measured, 4008 of them unique (R_{int} = 0.0458), with 2088 having I > 2σ(I). All 4098 reflections were used in the structure refinement based on F^2 by full-matrix least-squares techniques. The analysis of anisotropic displacement parameters as well as the Fourrier electron density synthesis have revealed that C(1), C(2), C(3) and C(10), C(11), C(12) atoms of rings are

disordered by two positions (with equal occupancies) due to the superposition of two chiral conformations. Hydrogen atoms in the ordered part were located from Fourrier electron density synthesis and included into refinement in isotropic approximation. The remainig hydrogen atoms in the disordered part were calculated in ideal positions, riding during refinement on the respective pivot atom. Their isotropic displacement parameters were set to 1.2 × U_{eq} of the attached atom. Final R_F = 0.0537 for observed data and wR2 = 0.1341 on F^2 for all data.

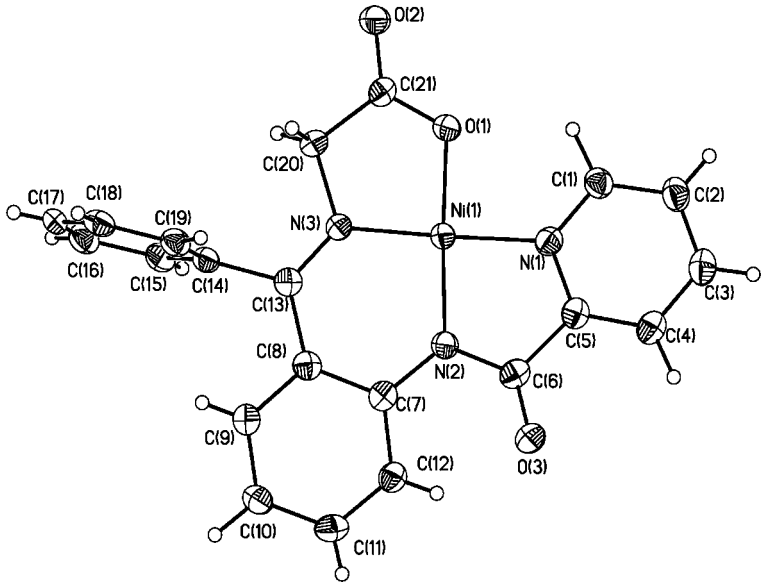

Figure S20. An ORTEP diagram of **1**. The thermal ellipsoids are drawn on 50% probability level.

Table S1. Crystal data and structure refinement for **1**.

Identification code	comp **1**	
Empirical formula	C21 H15 N3 Ni O3	
Formula weight	416.07	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.783(3) Å	α= 90°.
	b = 18.550(4) Å	β= 101.687(5)°.
	c = 7.2338(14) Å	γ = 90°.
Volume	1679.8(6) $Å^3$	
Z	4	
Density (calculated)	1.645 Mg/m^3	
Absorption coefficient	1.185 mm^{-1}	
F(000)	856	
Crystal size	0.35 x 0.32 x 0.25 mm^3	
Theta range for data collection	2.73 to 28.00°.	
Index ranges	-16<=h<=15, -24<=k<=11, -9<=l<=9	
Reflections collected	9250	
Independent reflections	3982 [R(int) = 0.0362]	
Completeness to theta = 28.00°	98.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.846 and 0.753	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3982 / 0 / 313	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0528, wR2 = 0.1150	
R indices (all data)	R1 = 0.0761, wR2 = 0.1228	
Largest diff. peak and hole	0.679 and -0.572 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	1589(1)	-8(1)	723(1)	23(1)
O(1)	1275(2)	-751(1)	2229(3)	29(1)
O(2)	1716(2)	-1877(1)	3126(3)	30(1)
O(3)	1715(2)	2026(1)	-613(3)	33(1)
N(1)	693(2)	620(1)	1717(4)	25(1)
N(2)	1835(2)	767(1)	-765(4)	24(1)
N(3)	2531(2)	-626(1)	-89(4)	23(1)
C(1)	60(3)	465(2)	2919(5)	28(1)
C(2)	-517(3)	995(2)	3627(5)	31(1)
C(3)	-441(3)	1696(2)	3080(5)	31(1)
C(4)	218(3)	1860(2)	1840(5)	29(1)
C(5)	762(3)	1312(2)	1172(5)	25(1)
C(6)	1486(3)	1418(2)	-186(5)	26(1)
C(7)	2368(3)	737(2)	-2267(4)	24(1)
C(8)	3000(3)	122(2)	-2528(4)	24(1)
C(9)	3557(3)	130(2)	-4021(5)	28(1)
C(10)	3488(3)	699(2)	-5263(5)	31(1)
C(11)	2843(3)	1281(2)	-5038(5)	30(1)
C(12)	2284(3)	1294(2)	-3593(5)	26(1)
C(13)	3101(3)	-521(2)	-1351(4)	23(1)
C(14)	3878(3)	-1092(2)	-1679(4)	24(1)
C(15)	3581(3)	-1593(2)	-3127(5)	25(1)
C(16)	4323(3)	-2104(2)	-3440(5)	29(1)
C(17)	5318(3)	-2121(2)	-2301(5)	26(1)
C(18)	5617(3)	-1633(2)	-867(5)	27(1)
C(19)	4888(3)	-1117(2)	-555(5)	27(1)
C(20)	2624(3)	-1322(2)	946(5)	27(1)
C(21)	1817(3)	-1335(2)	2196(4)	22(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Ni(1)-N(3)	1.843(2)
Ni(1)-O(1)	1.851(2)
Ni(1)-N(2)	1.861(3)
Ni(1)-N(1)	1.876(3)
O(1)-C(21)	1.289(4)
O(2)-C(21)	1.231(4)
O(3)-C(6)	1.220(4)
N(1)-C(1)	1.333(4)
N(1)-C(5)	1.352(4)
N(2)-C(6)	1.381(4)
N(2)-C(7)	1.395(4)
N(3)-C(13)	1.292(4)
N(3)-C(20)	1.486(4)
C(1)-C(2)	1.388(5)
C(2)-C(3)	1.368(5)
C(3)-C(4)	1.383(5)
C(4)-C(5)	1.374(4)
C(5)-C(6)	1.492(5)
C(7)-C(12)	1.399(4)
C(7)-C(8)	1.433(4)
C(8)-C(9)	1.408(5)
C(8)-C(13)	1.457(4)
C(9)-C(10)	1.377(5)
C(10)-C(11)	1.388(5)
C(11)-C(12)	1.381(5)
C(13)-C(14)	1.503(4)
C(14)-C(19)	1.381(5)
C(14)-C(15)	1.395(4)
C(15)-C(16)	1.392(5)
C(16)-C(17)	1.368(5)
C(17)-C(18)	1.372(5)
C(18)-C(19)	1.386(5)
C(20)-C(21)	1.503(4)
N(3)-Ni(1)-O(1)	87.62(10)
N(3)-Ni(1)-N(2)	95.63(11)
O(1)-Ni(1)-N(2)	176.67(11)
N(3)-Ni(1)-N(1)	176.00(11)

O(1)-Ni(1)-N(1)	90.82(11)
N(2)-Ni(1)-N(1)	85.99(11)
C(21)-O(1)-Ni(1)	115.7(2)
C(1)-N(1)-C(5)	118.7(3)
C(1)-N(1)-Ni(1)	127.9(2)
C(5)-N(1)-Ni(1)	113.4(2)
C(6)-N(2)-C(7)	120.6(3)
C(6)-N(2)-Ni(1)	113.4(2)
C(7)-N(2)-Ni(1)	125.9(2)
C(13)-N(3)-C(20)	119.1(3)
C(13)-N(3)-Ni(1)	129.1(2)
C(20)-N(3)-Ni(1)	111.76(19)
N(1)-C(1)-C(2)	121.7(3)
C(3)-C(2)-C(1)	119.5(3)
C(2)-C(3)-C(4)	119.0(3)
C(5)-C(4)-C(3)	118.9(3)
N(1)-C(5)-C(4)	122.1(3)
N(1)-C(5)-C(6)	113.8(3)
C(4)-C(5)-C(6)	124.1(3)
O(3)-C(6)-N(2)	128.4(3)
O(3)-C(6)-C(5)	120.1(3)
N(2)-C(6)-C(5)	111.5(3)
C(12)-C(7)-N(2)	121.5(3)
C(12)-C(7)-C(8)	117.7(3)
N(2)-C(7)-C(8)	120.8(3)
C(9)-C(8)-C(7)	118.6(3)
C(9)-C(8)-C(13)	117.3(3)
C(7)-C(8)-C(13)	124.1(3)
C(10)-C(9)-C(8)	122.2(3)
C(9)-C(10)-C(11)	118.7(3)
C(12)-C(11)-C(10)	120.9(3)
C(11)-C(12)-C(7)	121.8(3)
N(3)-C(13)-C(8)	122.7(3)
N(3)-C(13)-C(14)	119.4(3)
C(8)-C(13)-C(14)	117.9(3)
C(19)-C(14)-C(15)	120.0(3)
C(19)-C(14)-C(13)	120.0(3)
C(15)-C(14)-C(13)	120.0(3)
C(16)-C(15)-C(14)	119.0(3)
C(17)-C(16)-C(15)	119.9(3)

C(16)-C(17)-C(18)	121.5(3)
C(17)-C(18)-C(19)	119.0(3)
C(14)-C(19)-C(18)	120.4(3)
N(3)-C(20)-C(21)	108.8(3)
O(2)-C(21)-O(1)	124.0(3)
O(2)-C(21)-C(20)	120.2(3)
O(1)-C(21)-C(20)	115.8(3)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	28(1)	20(1)	23(1)	0(1)	9(1)	1(1)
O(1)	39(1)	23(1)	28(1)	2(1)	15(1)	1(1)
O(2)	38(1)	25(1)	28(1)	2(1)	10(1)	-1(1)
O(3)	43(2)	21(1)	38(1)	1(1)	15(1)	2(1)
N(1)	28(1)	23(1)	22(1)	0(1)	3(1)	2(1)
N(2)	31(2)	21(1)	22(1)	-2(1)	8(1)	-1(1)
N(3)	26(1)	19(1)	24(1)	0(1)	7(1)	0(1)
C(1)	28(2)	31(2)	24(2)	1(1)	5(2)	2(1)
C(2)	32(2)	35(2)	26(2)	-4(1)	8(2)	5(2)
C(3)	30(2)	34(2)	30(2)	-6(2)	5(2)	6(2)
C(4)	29(2)	27(2)	29(2)	-2(1)	1(2)	3(1)
C(5)	25(2)	25(2)	25(2)	-3(1)	3(1)	0(1)
C(6)	28(2)	23(2)	26(2)	0(1)	1(1)	-1(1)
C(7)	23(2)	24(2)	25(2)	-2(1)	2(1)	-1(1)
C(8)	27(2)	25(2)	19(2)	-3(1)	2(1)	-2(1)
C(9)	29(2)	28(2)	29(2)	-1(1)	8(2)	3(1)
C(10)	38(2)	31(2)	29(2)	2(1)	14(2)	-1(2)
C(11)	37(2)	27(2)	25(2)	4(1)	3(2)	-2(2)
C(12)	25(2)	26(2)	27(2)	1(1)	3(2)	3(1)
C(13)	24(2)	22(2)	21(2)	-3(1)	2(1)	-3(1)
C(14)	28(2)	21(2)	24(2)	1(1)	11(1)	-2(1)
C(15)	27(2)	29(2)	20(2)	-1(1)	5(2)	-3(1)
C(16)	38(2)	28(2)	24(2)	-4(1)	12(2)	-5(1)
C(17)	30(2)	24(2)	27(2)	4(1)	16(2)	3(1)
C(18)	25(2)	31(2)	27(2)	6(1)	8(2)	-4(1)
C(19)	34(2)	25(2)	23(2)	-2(1)	9(2)	-4(1)
C(20)	33(2)	20(2)	30(2)	4(1)	10(2)	3(1)
C(21)	26(2)	19(1)	19(2)	-5(1)	-1(1)	-1(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

	x	y	z	U(eq)
H(2)	-970(30)	884(16)	4370(40)	14(8)
H(3)	-920(30)	2005(19)	3390(50)	29(9)
H(4)	300(30)	2382(18)	1620(40)	22(8)
H(9)	3940(30)	-222(18)	-4170(50)	20(9)
H(10)	3940(30)	706(18)	-6180(50)	29(9)
H(11)	2740(30)	1617(19)	-5760(50)	26(9)
H(12)	1860(30)	1620(20)	-3500(50)	31(10)
H(19)	2880(30)	-1580(18)	-3880(50)	26(9)
H(16)	4110(30)	-2450(20)	-4470(50)	34(10)
H(17)	5760(30)	-2380(20)	-2420(60)	44(12)
H(18)	6300(30)	-1645(17)	-150(50)	23(9)
H(19)	5110(30)	-860(20)	430(50)	39(11)
H(20B)	2530(30)	-1730(20)	140(50)	37(10)
H(20A)	3300(30)	-1374(16)	1720(50)	17(8)
H(1)	60(30)	-87(18)	3260(50)	31(10)

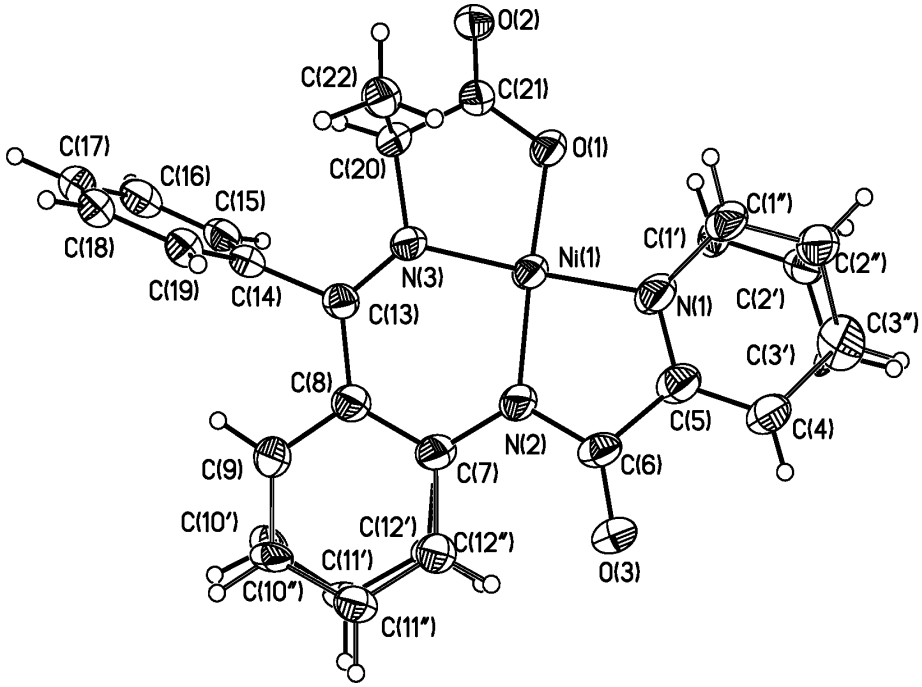

Figure S21. An ORTEP diagram of **2** (two positions of disodered rings are shown). The thermal ellipsoids are drawn on 50% probability level.

Table S6. Crystal data and structure refinement for **2**.

Identification code	comp **2**	
Empirical formula	C22 H17 N3 Ni O3	
Formula weight	430.10	
Temperature	110(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 7.987(4) Å	α= 90°.
	b = 21.557(10)Å	β= 110.403(9)°.
	c = 10.936(5) Å	γ = 90°.
Volume	1764.9(14) $Å^3$	
Z	4	
Density (calculated)	1.619 Mg/m^3	
Absorption coefficient	1.131 mm^{-1}	
F(000)	888	
Crystal size	0.40 x 0.30 x 0.20 mm^3	
Theta range for data collection	2.74 to 27.55°.	
Index ranges	-10<=h<=10, -28<=k<=27, -14<=l<=13	
Reflections collected	10376	
Independent reflections	4008 [R(int) = 0.0458]	
Completeness to theta = 27.55°	98.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4008 / 0 / 360	
Goodness-of-fit on F^2	0.935	
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1161	
R indices (all data)	R1 = 0.1058, wR2 = 0.1341	
Largest diff. peak and hole	0.823 and -0.744 $e.E^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni(1)	2109(1)	513(1)	3489(1)	48(1)
O(1)	1437(4)	873(1)	1846(2)	44(1)
O(2)	245(3)	1738(1)	785(2)	36(1)
O(3)	3612(4)	-903(1)	5887(2)	47(1)
N(1)	2779(6)	-219(1)	2844(3)	68(1)
N(2)	2582(4)	79(1)	5059(3)	44(1)
N(3)	1588(4)	1264(1)	4084(3)	31(1)
C(1')*	2282(12)	-374(4)	1568(8)	33(2)
C(2')*	2834(13)	-951(4)	1266(9)	37(2)
C(3')*	3750(40)	-1354(7)	2250(30)	54(7)
C(1")*	3369(13)	-250(4)	1715(8)	39(2)
C(2")*	3785(14)	-819(4)	1304(9)	41(2)
C(3")*	3920(40)	-1350(11)	2120(20)	61(8)
C(4)	3810(5)	-1250(2)	3423(4)	41(1)
C(5)	3265(5)	-673(2)	3711(3)	41(1)
C(6)	3187(5)	-513(2)	5027(3)	34(1)
C(7)	2262(7)	301(2)	6162(4)	57(1)
C(8)	1587(5)	918(2)	6191(3)	40(1)
C(9)	1222(6)	1102(2)	7305(4)	42(1)
C(10")*	1048(18)	727(9)	8221(17)	42(4)
C(11")*	1488(12)	121(4)	8202(7)	35(2)
C(12")*	1935(12)	-103(3)	7153(8)	32(2)
C(10')*	1843(17)	739(8)	8474(17)	40(4)
C(11')*	2754(13)	166(4)	8475(8)	44(2)
C(12')*	3099(13)	-35(4)	7394(8)	38(2)
C(13)	1327(4)	1380(1)	5168(3)	29(1)
C(14)	716(5)	2019(2)	5381(3)	29(1)
C(15)	-1085(5)	2168(2)	4829(3)	34(1)
C(16)	-1668(6)	2764(2)	4985(4)	39(1)
C(17)	-467(6)	3204(2)	5708(4)	40(1)
C(18)	1325(6)	3057(2)	6259(4)	36(1)
C(19)	1913(6)	2467(2)	6094(3)	33(1)
C(20)	1430(5)	1765(1)	3116(3)	30(1)
C(21)	944(5)	1450(2)	1791(3)	31(1)
C(22)	3194(6)	2102(2)	3413(4)	35(1)

*Atom in the disordered rings is refined with occupancy 0.5.

Table S8. Bond lengths [Å] and angles [°] for **2**.

Ni(1)-N(3)	1.846(3)
Ni(1)-O(1)	1.857(2)
Ni(1)-N(2)	1.874(3)
Ni(1)-N(1)	1.881(3)
O(1)-C(21)	1.299(4)
O(2)-C(21)	1.217(4)
O(3)-C(6)	1.217(4)
N(1)-C(5)	1.323(4)
N(1)-C(1')	1.353(8)
N(1)-C(1")	1.469(9)
N(2)-C(6)	1.370(4)
N(2)-C(7)	1.402(5)
N(3)-C(13)	1.297(4)
N(3)-C(20)	1.486(4)
C(1')-C(2')	1.397(11)
C(2')-C(3')	1.38(2)
C(3')-C(4)	1.29(3)
C(1")-C(2")	1.386(11)
C(2")-C(3")	1.43(3)
C(3")-C(4)	1.48(3)
C(4)-C(5)	1.388(5)
C(5)-C(6)	1.503(5)
C(7)-C(8)	1.439(5)
C(7)-C(12')	1.469(9)
C(7)-C(12")	1.483(8)
C(8)-C(9)	1.405(5)
C(8)-C(13)	1.456(4)
C(9)-C(10")	1.33(2)
C(9)-C(10')	1.431(17)
C(10")-C(11")	1.35(2)
C(11")-C(12")	1.401(11)
C(10')-C(11')	1.43(2)
C(11')-C(12')	1.374(11)
C(13)-C(14)	1.507(4)
C(14)-C(15)	1.390(5)
C(14)-C(19)	1.392(5)
C(15)-C(16)	1.396(5)
C(16)-C(17)	1.385(5)

C(17)-C(18)	1.382(5)
C(18)-C(19)	1.388(5)
C(20)-C(22)	1.517(5)
C(20)-C(21)	1.523(4)

N(3)-Ni(1)-O(1)	87.12(11)
N(3)-Ni(1)-N(2)	96.51(12)
O(1)-Ni(1)-N(2)	173.27(12)
N(3)-Ni(1)-N(1)	175.42(15)
O(1)-Ni(1)-N(1)	90.68(12)
N(2)-Ni(1)-N(1)	86.09(13)
C(21)-O(1)-Ni(1)	115.2(2)
C(5)-N(1)-C(1')	117.6(4)
C(5)-N(1)-C(1")	118.0(4)
C(1')-N(1)-C(1")	35.5(4)
C(5)-N(1)-Ni(1)	113.8(3)
C(1')-N(1)-Ni(1)	125.0(4)
C(1")-N(1)-Ni(1)	124.7(4)
C(6)-N(2)-C(7)	120.8(3)
C(6)-N(2)-Ni(1)	113.8(2)
C(7)-N(2)-Ni(1)	125.4(2)
C(13)-N(3)-C(20)	120.8(3)
C(13)-N(3)-Ni(1)	128.1(2)
C(20)-N(3)-Ni(1)	111.0(2)
N(1)-C(1')-C(2')	117.4(7)
C(3')-C(2')-C(1')	120.2(13)
C(4)-C(3')-C(2')	119.6(18)
C(2")-C(1")-N(1)	119.7(7)
C(1")-C(2")-C(3")	118.9(14)
C(2")-C(3")-C(4)	117.7(17)
C(3')-C(4)-C(5)	118.5(8)
C(5)-C(4)-C(3")	118.7(10)
N(1)-C(5)-C(4)	122.4(4)
N(1)-C(5)-C(6)	114.6(3)
C(4)-C(5)-C(6)	123.0(3)
O(3)-C(6)-N(2)	129.0(3)
O(3)-C(6)-C(5)	119.2(3)
N(2)-C(6)-C(5)	111.8(3)
N(2)-C(7)-C(8)	121.1(3)
N(2)-C(7)-C(12')	117.4(5)

C(8)-C(7)-C(12')	119.3(4)
N(2)-C(7)-C(12")	124.0(4)
C(8)-C(7)-C(12")	111.4(4)
C(12')-C(7)-C(12")	34.9(4)
C(9)-C(8)-C(7)	118.2(3)
C(9)-C(8)-C(13)	117.1(3)
C(7)-C(8)-C(13)	124.7(3)
C(10")-C(9)-C(8)	126.0(9)
C(10")-C(9)-C(10')	24.7(8)
C(8)-C(9)-C(10')	120.6(9)
C(9)-C(10")-C(11")	118.6(16)
C(10")-C(11")-C(12")	119.1(11)
C(11")-C(12")-C(7)	123.7(6)
C(9)-C(10')-C(11')	119.3(15)
C(12')-C(11')-C(10')	121.6(10)
C(11')-C(12')-C(7)	118.1(8)
N(3)-C(13)-C(8)	123.1(3)
N(3)-C(13)-C(14)	118.6(3)
C(8)-C(13)-C(14)	118.3(3)
C(15)-C(14)-C(19)	119.2(3)
C(15)-C(14)-C(13)	119.1(3)
C(19)-C(14)-C(13)	121.7(3)
C(14)-C(15)-C(16)	119.9(4)
C(17)-C(16)-C(15)	120.4(4)
C(18)-C(17)-C(16)	119.9(4)
C(17)-C(18)-C(19)	119.9(4)
C(18)-C(19)-C(14)	120.7(4)
N(3)-C(20)-C(22)	110.7(3)
N(3)-C(20)-C(21)	106.5(2)
C(22)-C(20)-C(21)	109.1(3)
O(2)-C(21)-O(1)	124.6(3)
O(2)-C(21)-C(20)	121.1(3)
O(1)-C(21)-C(20)	114.2(3)

Table S9. Anisotropic displacement parameters ($E^2 x 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni(1)	94(1)	23(1)	25(1)	1(1)	19(1)	9(1)
O(1)	78(2)	24(1)	28(1)	0(1)	15(1)	6(1)
O(2)	41(2)	37(1)	28(1)	7(1)	10(1)	7(1)
O(3)	62(2)	37(1)	44(2)	16(1)	21(1)	15(1)
N(1)	140(4)	29(2)	29(2)	2(1)	21(2)	23(2)
N(2)	80(3)	22(2)	27(2)	-2(1)	14(2)	2(2)
N(3)	42(2)	25(1)	25(2)	2(1)	9(1)	1(1)
C(1')*	45(5)	25(4)	25(4)	-4(3)	7(4)	6(4)
C(2')*	60(7)	25(4)	27(4)	-6(3)	19(5)	-12(4)
C(3')*	97(14)	8(6)	61(14)	-3(6)	33(11)	15(6)
C(1")*	55(6)	22(4)	36(5)	-2(3)	10(5)	-6(4)
C(2")*	58(7)	32(5)	33(5)	-1(4)	14(5)	-1(5)
C(3")*	76(14)	67(13)	17(7)	-16(6)	-15(10)	19(9)
C(4)	54(3)	28(2)	33(2)	2(2)	2(2)	2(2)
C(5)	53(3)	29(2)	31(2)	1(2)	3(2)	-2(2)
C(6)	41(2)	24(2)	29(2)	4(2)	3(2)	-6(2)
C(7)	114(4)	25(2)	32(2)	3(2)	25(2)	2(2)
C(8)	59(3)	29(2)	30(2)	-1(2)	14(2)	-7(2)
C(9)	64(3)	27(2)	35(2)	-5(2)	18(2)	-9(2)
C(10")*	59(10)	37(5)	21(7)	-13(5)	4(7)	-17(8)
C(11")*	40(5)	38(4)	20(4)	9(3)	2(4)	-5(4)
C(12")*	51(6)	18(3)	24(4)	2(3)	10(5)	1(4)
C(10')*	69(10)	25(4)	13(6)	0(4)	-2(7)	-18(8)
C(11')*	65(6)	37(4)	26(4)	3(3)	12(5)	-1(5)
C(12')*	53(6)	30(4)	31(5)	-1(3)	13(5)	-3(4)
C(13)	35(2)	28(2)	23(2)	-1(1)	7(2)	-5(2)
C(14)	38(2)	30(2)	21(2)	3(1)	12(2)	1(2)
C(15)	40(2)	39(2)	23(2)	1(2)	11(2)	-3(2)
C(16)	37(3)	52(2)	28(2)	6(2)	14(2)	9(2)
C(17)	57(3)	34(2)	33(2)	4(2)	23(2)	9(2)
C(18)	53(3)	32(2)	27(2)	-2(2)	16(2)	-2(2)
C(19)	40(3)	34(2)	25(2)	-1(2)	11(2)	-1(2)
C(20)	37(2)	23(2)	29(2)	4(1)	12(2)	2(2)
C(21)	38(2)	27(2)	30(2)	0(2)	15(2)	-2(2)
C(22)	47(3)	31(2)	26(2)	-3(2)	11(2)	-4(2)

*Atom in the disordered rings is refined with occupancy 0.5.

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(1'A)*	1584	-101	904	40
H(2'A)*	2580	-1065	380	44
H(3'A)*	4324	-1708	2060	65
H(1"A)*	3464	119	1268	47
H(2"A)*	3977	-855	497	50
H(3"A)*	4075	-1754	1824	74
H(10A)*	625	881	8874	50
H(11A)*	1494	-148	8891	42
H(12A)*	2034	-539	7071	38
H(10B)*	1653	877	9241	49
H(11B)*	3129	-81	9243	52
H(12B)*	3855	-381	7442	46
H(22C)	3600(40)	2333(14)	4250(30)	31(9)
H(22B)	4170(50)	1805(17)	3520(40)	49(11)
H(22A)	3100(40)	2358(14)	2770(30)	25(9)
H(9)	790(40)	1522(17)	7280(30)	40(10)
H(4)	4120(50)	-1546(16)	3960(30)	38(10)
H(15)	-1830(50)	1883(15)	4310(30)	32(10)
H(20)	490(40)	2078(14)	3100(30)	30(9)
H(11)	-2760(40)	2852(14)	4610(30)	19(9)
H(17)	-920(40)	3641(16)	5820(30)	43(10)
H(19)	3040(40)	2384(14)	6440(30)	24(10)
H(18)	2210(50)	3362(18)	6800(40)	53(11)

*Atom in the disordered rings is refined with occupancy 0.5.

The X-ray data for **32b**, **32d**, and **32f** were obtained at 150 K using Oxford Cryostream low-temperature device on a Nonius KappaCCD diffractometer with Mo K_α radiation (λ = 0.71069 Å), a graphite monochromator, and the φ and ω scan mode. Data reduction was performed with DENZO-SMN (Otwinowski, Z.; Minor, W. *Methods Enzymol.* Part A **1977**, *276*, 307). Structures were solved by direct methods [Sir92 (Altomare, A.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Burla, M.C.; Polidori, G.; Camalli, M. *J. Appl. Cryst.* **1994**, *27*, 435.)] and refined by full matrix least-square (Sheldrick, G. M. SHELXL97. University of Göttingen, Germany).

Crystal data for (*R*)-**32b**: $C_{22}H_{17}NO_2$, M = 327.37. Crystals were obtained from toluene; they are orthorhombic, of space group $P2_12_12_1$, with a = 13.7530(3) Å, b = 14.1390(3) Å, c = 17.5720(3) Å, V = 3416.94(12) Å^3, Z = 8, d_{calc} = 1.273 g cm^{-3}, μ = 0.082 mm^{-1}. A total of 28631 reflections were measured, 7493 of them unique (R_{int} = 0.025), with 6690 having I > 2σ(I). All 7493 reflections were used in the structure refinement based on F^2 by full-matrix least-squares techniques. Hydrogen atoms on carbon were calculated in ideal positions, riding during refinement on the respective pivot atom (469 parameters). The isotropic displacement parameters of hydrogen atoms on C were set to 1.2 x U_{eq} of the attached atom (1.5 x U_{eq} for methyl hydrogen atoms). Hydrogen atoms on O and N were found on difference Fourier map and refined isotropicaly. Final R_F = 0.043 for observed data and R_w = 0.103 on F^2 for all data.

Crystal data for (*S*)-**32d**: $C_{25}H_{23}NO_2$, M = 369.44. Crystals were obtained from toluene; they are monoclinic, of space group $P2_1$, with a = 7.7500(2) Å, b = 9.6320(2) Å, c = 13.4030(3) Å, β = 102.561(2)° , V = 976.56(4) Å^3, Z = 2, d_{calc} = 1.256 g cm^{-3}, μ = 0.079 mm^{-1}. A total of 15820 reflections were measured, 4446 of them unique (R_{int} = 0.030), with 4195 having I > 2σ(I). All 4446 reflections were used in the structure refinement based on F^2 by full-matrix least-squares techniques. Hydrogen atoms on carbon were calculated in ideal positions, riding during refinement on the respective pivot atom (264 parameters). Their isotropic displacement parameters were set to 1.2 x U_{eq} of the attached atom (1.5 x U_{eq} for methyl hydrogen atoms). Hydrogen atoms on O and N were found on difference Fourier map and refined isotropicaly. Final R_F = 0.035 for observed data and R_w = 0.089 on F^2 for all data.

Crystal data for (*R*)-**32f**: $C_{31}H_{29}NO_2$, M = 447.55. Crystals were obtained from ?????; they are monoclinic, of space group $P2_1$, with a = 11.1730(2) Å, b = 8.9400(2) Å, c = 11.6690(2) Å, β = 98.011(1)°, V = 1154.20(4) Å^3, Z = 2, d_{calc} = 1.288 g cm^{-3}, μ = 0.080 mm^{-1}. A total of 17572 reflections were measured, 5180 of them unique (R_{int} = 0.027), with 4888 having I > 2σ(I). All 5180 reflections were used in the structure refinement based on F^2 by full-matrix least-squares techniques. Hydrogen atoms on carbon were calculated in ideal positions, riding during refinement on the respective pivot atom (315 parameters). The isotropic displacement parameters of this hydrogen atoms were set to 1.2 x U_{eq} of the attached carbon atom. Hydrogen atoms on O and N were found on difference Fourier map and refined isotropically. Final R_F = 0.033 for observed data and R_w = 0.081 on F^2 for all data.

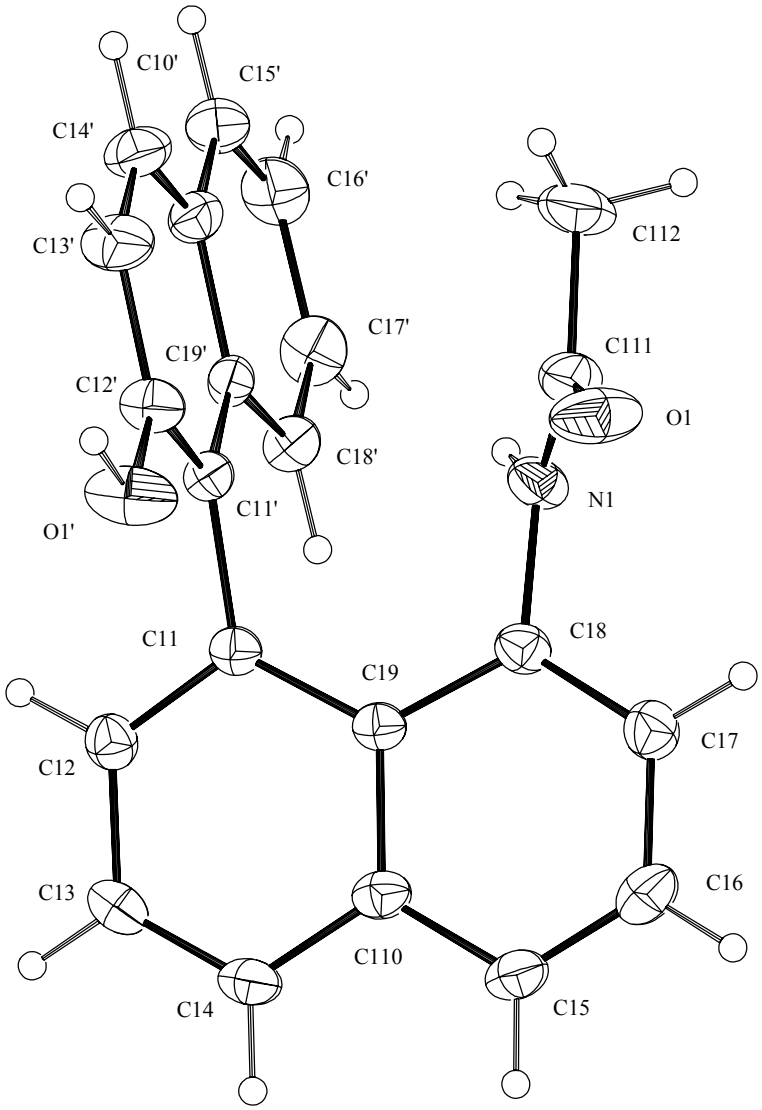

Figure S22. An ORTEP diagram of (*R*)-**32b** (rotamer A). The thermal ellipsoids are drawn on 30% probability level.

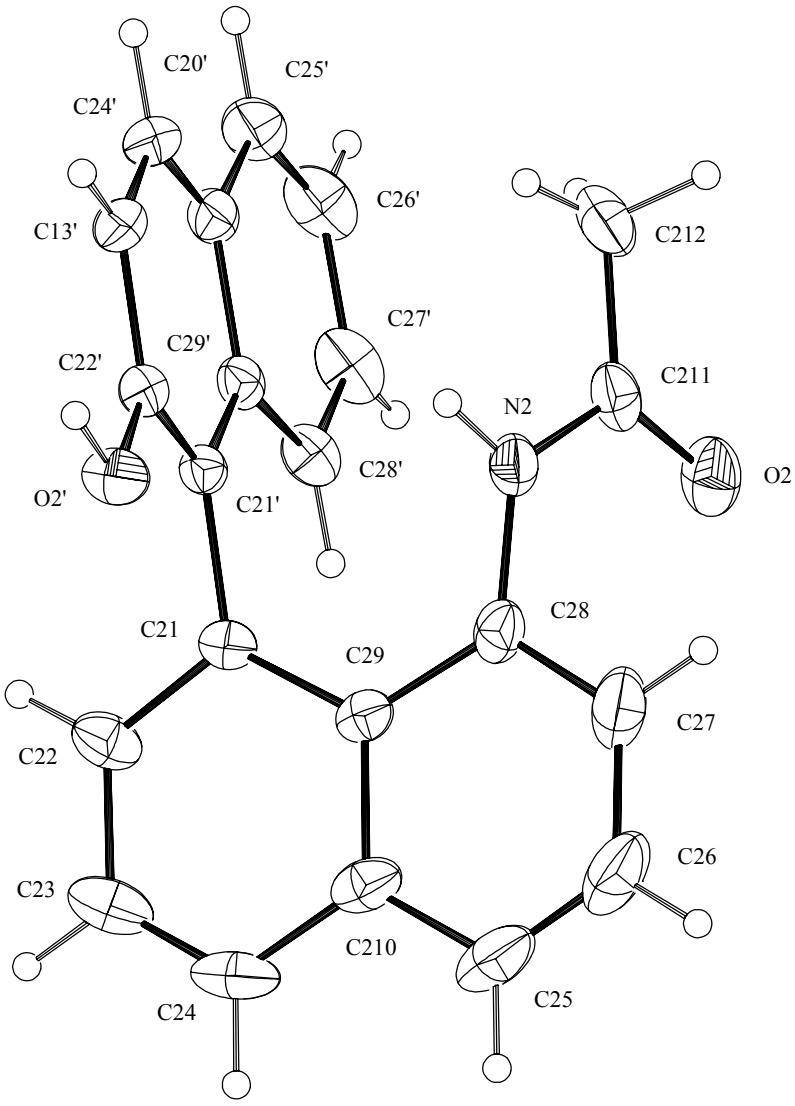

Figure S23. An ORTEP diagram of (*R*)-**32b** (rotamer **B**). The thermal ellipsoids are drawn on 30% probability level.

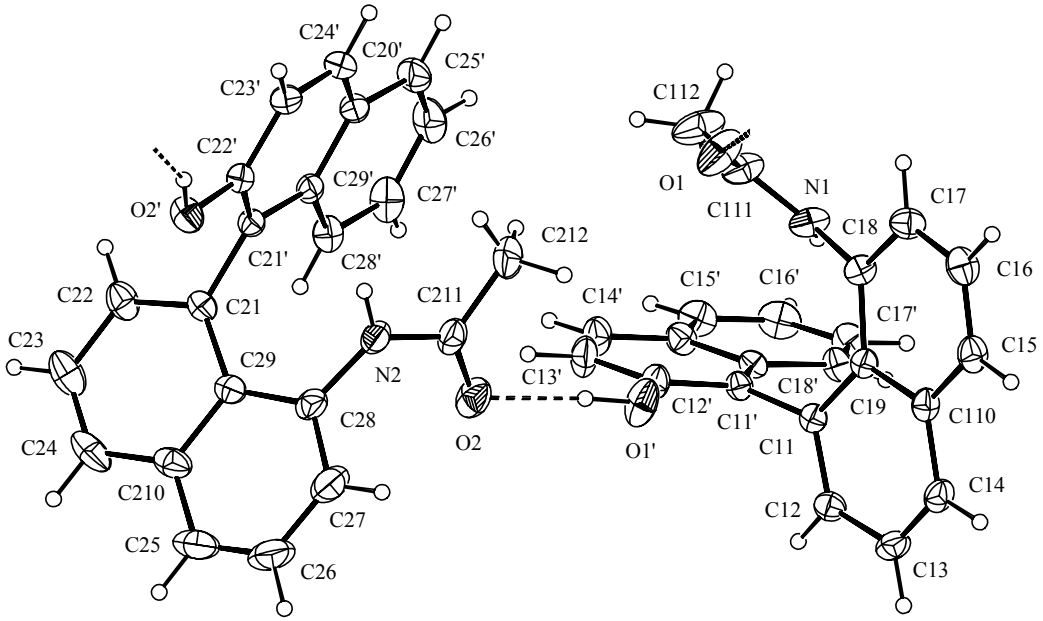

Figure S24. An ORTEP diagram of (*R*)-**32b** (rotamers **A** and **B** connected by hydrogen bonding). The thermal ellipsoids are drawn on 30% probability level.

Table S11. Crystal data and structure refinement for **32b**.

Identification code	**32b**
Empirical formula	C22 H17 N O2
Formula weight	327.37
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Orthorhombic, P 21 21 21
Unit cell dimensions	a = 13.7530(3) A alpha = 90 deg. b = 14.1390(3) A beta = 90 deg. c = 17.5720(3) A gamma = 90 deg.
Volume	3416.94(12) A^3
Z, Calculated density	8, 1.273 Mg/m^3
Absorption coefficient	0.082 mm^-1
F(000)	1376
Crystal size	0.35 x 0.3 x 0.22 mm
Theta range for data collection	2.75 to 27.11 deg.
Limiting indices	-17<=h<=17, -18<=k<=18, -22<=l<=22
Reflections collected / unique	28631 / 7493 [R(int) = 0.0250]
Completeness to theta = 27.11	99.4 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7493 / 0 / 469
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0434, wR2 = 0.0985
R indices (all data)	R1 = 0.0518, wR2 = 0.1030
Absolute structure parameter	-0.2(10)
Largest diff. peak and hole	0.174 and -0.212 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **32b**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(11)	12141(1)	706(1)	5041(1)	30(1)
C(12)	12918(1)	1289(1)	5183(1)	37(1)
C(13)	12809(1)	2181(1)	5527(1)	43(1)
C(14)	11911(1)	2483(1)	5743(1)	42(1)
C(15)	10158(1)	2242(1)	5854(1)	44(1)
C(16)	9346(1)	1727(1)	5713(1)	48(1)
C(17)	9410(1)	886(1)	5293(1)	43(1)
C(18)	10293(1)	550(1)	5052(1)	36(1)
C(19)	11179(1)	1032(1)	5224(1)	31(1)
C(110)	11084(1)	1923(1)	5608(1)	36(1)
C(111)	9985(1)	-1137(1)	4804(1)	51(1)
C(112)	10096(2)	-1906(2)	4217(2)	74(1)
N(1)	10306(1)	-282(1)	4592(1)	42(1)
O(1)	9614(1)	-1288(1)	5425(1)	72(1)
O(1')	12430(1)	-873(1)	5963(1)	63(1)
C(11')	12367(1)	-258(1)	4727(1)	31(1)
C(12')	12533(1)	-1009(1)	5205(1)	41(1)
C(13')	12804(2)	-1906(1)	4916(1)	52(1)
C(14')	12914(2)	-2048(1)	4160(1)	50(1)
C(15')	12865(2)	-1426(2)	2842(1)	50(1)
C(16')	12691(2)	-706(2)	2354(1)	54(1)
C(17')	12400(2)	174(2)	2633(1)	51(1)
C(18')	12298(1)	325(1)	3397(1)	38(1)
C(19')	12477(1)	-402(1)	3927(1)	31(1)
C(10')	12751(1)	-1309(1)	3641(1)	39(1)
C(21)	8023(1)	377(1)	2547(1)	34(1)
C(22)	8468(2)	1234(2)	2673(1)	49(1)
C(23)	9418(2)	1424(2)	2432(1)	64(1)
C(24)	9928(2)	758(2)	2062(1)	63(1)
C(25)	10055(2)	-841(2)	1507(1)	70(1)
C(26)	9663(2)	-1686(2)	1334(2)	80(1)
C(27)	8724(2)	-1914(2)	1589(1)	67(1)
C(28)	8190(1)	-1283(1)	2007(1)	42(1)
C(29)	8556(1)	-358(1)	2167(1)	36(1)
C(210)	9527(1)	-150(2)	1918(1)	49(1)
C(211)	7133(2)	-2214(1)	2844(1)	46(1)
C(212)	6106(2)	-2382(2)	3074(2)	72(1)
C(21')	6976(1)	289(1)	2765(1)	31(1)
C(22')	6275(1)	462(1)	2222(1)	36(1)
C(23')	5275(1)	379(1)	2397(1)	45(1)
C(24')	4989(1)	149(1)	3112(1)	49(1)
C(25')	5386(2)	-320(1)	4433(1)	55(1)
C(26')	6063(2)	-542(2)	4968(1)	60(1)
C(27')	7056(2)	-492(1)	4797(1)	54(1)
C(28')	7368(1)	-215(1)	4085(1)	42(1)
C(29')	6685(1)	24(1)	3515(1)	34(1)
C(20')	5674(1)	-37(1)	3690(1)	41(1)
N(2)	7263(1)	-1580(1)	2276(1)	43(1)
O(2)	7829(1)	-2617(1)	3147(1)	58(1)
O(2')	6578(1)	670(1)	1503(1)	46(1)

Table S13. Bond lengths [A] and angles [deg] for **32b**

C(11)-C(12)	1.372(2)
C(11)-C(19)	1.437(2)
C(11)-C(11')	1.504(2)
C(12)-C(13)	1.408(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.360(3)
C(13)-H(13)	0.9300
C(14)-C(110)	1.406(2)
C(14)-H(14)	0.9300
C(15)-C(16)	1.356(3)
C(15)-C(110)	1.420(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.403(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.371(2)
C(17)-H(17)	0.9300
C(18)-N(1)	1.428(2)
C(18)-C(19)	1.429(2)
C(19)-C(110)	1.434(2)
C(111)-O(1)	1.223(3)
C(111)-N(1)	1.340(3)
C(111)-C(112)	1.506(3)
C(112)-H(11A)	0.9600
C(112)-H(11B)	0.9600
C(112)-H(11C)	0.9600
N(1)-H(1)	0.84(2)
O(1')-C(12')	1.353(2)
O(1')-H(1')	0.90(3)
C(11')-C(12')	1.373(2)
C(11')-C(19')	1.427(2)
C(12')-C(13')	1.417(3)
C(13')-C(14')	1.351(3)
C(13')-H(13')	0.9300
C(14')-C(10')	1.405(3)
C(14')-H(14')	0.9300
C(15')-C(16')	1.353(3)
C(15')-C(10')	1.421(3)
C(15')-H(15')	0.9300
C(16')-C(17')	1.396(3)
C(16')-H(16')	0.9300
C(17')-C(18')	1.366(3)
C(17')-H(17')	0.9300
C(18')-C(19')	1.409(2)
C(18')-H(18')	0.9300
C(19')-C(10')	1.429(2)
C(21)-C(22)	1.375(2)
C(21)-C(29)	1.436(2)
C(21)-C(21')	1.496(2)
C(22)-C(23)	1.399(3)
C(22)-H(22)	0.9300
C(23)-C(24)	1.342(4)
C(23)-H(23)	0.9300
C(24)-C(210)	1.421(3)
C(24)-H(24)	0.9300
C(25)-C(26)	1.346(4)
C(25)-C(210)	1.415(3)
C(25)-H(25)	0.9300
C(26)-C(27)	1.404(4)
C(26)-H(26)	0.9300
C(27)-C(28)	1.370(3)

C(27)-H(27)	0.9300
C(28)-N(2)	1.422(3)
C(28)-C(29)	1.429(3)
C(29)-C(210)	1.435(2)
C(211)-O(2)	1.236(2)
C(211)-N(2)	1.353(2)
C(211)-C(212)	1.489(3)
C(212)-H(21A)	0.9600
C(212)-H(21B)	0.9600
C(212)-H(21C)	0.9600
C(21')-C(22')	1.378(2)
C(21')-C(29')	1.426(2)
C(22')-O(2')	1.364(2)
C(22')-C(23')	1.414(2)
C(23')-C(24')	1.356(3)
C(23')-H(23')	0.9300
C(24')-C(20')	1.411(3)
C(24')-H(24')	0.9300
C(25')-C(26')	1.360(3)
C(25')-C(20')	1.421(3)
C(25')-H(25')	0.9300
C(26')-C(27')	1.401(3)
C(26')-H(26')	0.9300
C(27')-C(28')	1.380(3)
C(27')-H(27')	0.9300
C(28')-C(29')	1.414(2)
C(28')-H(28')	0.9300
C(29')-C(20')	1.427(2)
N(2)-H(2)	0.83(2)
O(2')-H(2')	0.85(3)

C(12)-C(11)-C(19)	118.96(14)
C(12)-C(11)-C(11')	116.72(14)
C(19)-C(11)-C(11')	124.28(14)
C(11)-C(12)-C(13)	122.21(16)
C(11)-C(12)-H(12)	118.9
C(13)-C(12)-H(12)	118.9
C(14)-C(13)-C(12)	119.86(16)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(13)-C(14)-C(110)	120.67(15)
C(13)-C(14)-H(14)	119.7
C(110)-C(14)-H(14)	119.7
C(16)-C(15)-C(110)	120.83(16)
C(16)-C(15)-H(15)	119.6
C(110)-C(15)-H(15)	119.6
C(15)-C(16)-C(17)	119.99(17)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(18)-C(17)-C(16)	120.80(17)
C(18)-C(17)-H(17)	119.6
C(16)-C(17)-H(17)	119.6
C(17)-C(18)-N(1)	118.10(15)
C(17)-C(18)-C(19)	121.65(15)
N(1)-C(18)-C(19)	120.19(14)
C(18)-C(19)-C(110)	116.17(14)
C(18)-C(19)-C(11)	125.76(14)
C(110)-C(19)-C(11)	118.07(14)
C(14)-C(110)-C(15)	119.69(15)
C(14)-C(110)-C(19)	120.03(15)
C(15)-C(110)-C(19)	120.28(16)
O(1)-C(111)-N(1)	122.95(17)
O(1)-C(111)-C(112)	121.80(19)
N(1)-C(111)-C(112)	115.24(19)

C(111)-C(112)-H(11A)	109.5
C(111)-C(112)-H(11B)	109.5
H(11A)-C(112)-H(11B)	109.5
C(111)-C(112)-H(11C)	109.5
H(11A)-C(112)-H(11C)	109.5
H(11B)-C(112)-H(11C)	109.5
C(111)-N(1)-C(18)	125.50(15)
C(111)-N(1)-H(1)	119.8(16)
C(18)-N(1)-H(1)	113.6(16)
C(12')-O(1')-H(1')	112.8(18)
C(12')-C(11')-C(19')	118.35(15)
C(12')-C(11')-C(11)	120.69(14)
C(19')-C(11')-C(11)	120.84(13)
O(1')-C(12')-C(11')	118.38(15)
O(1')-C(12')-C(13')	120.50(16)
C(11')-C(12')-C(13')	121.12(16)
C(14')-C(13')-C(12')	120.92(17)
C(14')-C(13')-H(13')	119.5
C(12')-C(13')-H(13')	119.5
C(13')-C(14')-C(10')	120.71(17)
C(13')-C(14')-H(14')	119.6
C(10')-C(14')-H(14')	119.6
C(16')-C(15')-C(10')	121.29(18)
C(16')-C(15')-H(15')	119.4
C(10')-C(15')-H(15')	119.4
C(15')-C(16')-C(17')	119.90(17)
C(15')-C(16')-H(16')	120.1
C(17')-C(16')-H(16')	120.1
C(18')-C(17')-C(16')	120.92(19)
C(18')-C(17')-H(17')	119.5
C(16')-C(17')-H(17')	119.5
C(17')-C(18')-C(19')	121.19(17)
C(17')-C(18')-H(18')	119.4
C(19')-C(18')-H(18')	119.4
C(18')-C(19')-C(11')	121.91(15)
C(18')-C(19')-C(10')	117.89(14)
C(11')-C(19')-C(10')	120.18(14)
C(14')-C(10')-C(15')	122.50(17)
C(14')-C(10')-C(19')	118.71(15)
C(15')-C(10')-C(19')	118.78(16)
C(22)-C(21)-C(29)	119.01(16)
C(22)-C(21)-C(21')	117.45(16)
C(29)-C(21)-C(21')	123.37(14)
C(21)-C(22)-C(23)	122.5(2)
C(21)-C(22)-H(22)	118.8
C(23)-C(22)-H(22)	118.8
C(24)-C(23)-C(22)	119.9(2)
C(24)-C(23)-H(23)	120.0
C(22)-C(23)-H(23)	120.0
C(23)-C(24)-C(210)	121.16(18)
C(23)-C(24)-H(24)	119.4
C(210)-C(24)-H(24)	119.4
C(26)-C(25)-C(210)	121.5(2)
C(26)-C(25)-H(25)	119.3
C(210)-C(25)-H(25)	119.3
C(25)-C(26)-C(27)	120.0(2)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(28)-C(27)-C(26)	120.9(2)
C(28)-C(27)-H(27)	119.5
C(26)-C(27)-H(27)	119.5
C(27)-C(28)-N(2)	117.76(19)
C(27)-C(28)-C(29)	120.85(19)
N(2)-C(28)-C(29)	121.39(15)

C(28)-C(29)-C(210)	117.11(17)
C(28)-C(29)-C(21)	124.99(15)
C(210)-C(29)-C(21)	117.90(16)
C(25)-C(210)-C(24)	121.0(2)
C(25)-C(210)-C(29)	119.4(2)
C(24)-C(210)-C(29)	119.51(19)
O(2)-C(211)-N(2)	121.44(19)
O(2)-C(211)-C(212)	122.92(18)
N(2)-C(211)-C(212)	115.6(2)
C(211)-C(212)-H(21A)	109.5
C(211)-C(212)-H(21B)	109.5
H(21A)-C(212)-H(21B)	109.5
C(211)-C(212)-H(21C)	109.5
H(21A)-C(212)-H(21C)	109.5
H(21B)-C(212)-H(21C)	109.5
C(22')-C(21')-C(29')	119.34(14)
C(22')-C(21')-C(21)	118.81(14)
C(29')-C(21')-C(21)	121.86(14)
O(2')-C(22')-C(21')	117.78(15)
O(2')-C(22')-C(23')	121.09(16)
C(21')-C(22')-C(23')	121.06(16)
C(24')-C(23')-C(22')	120.15(18)
C(24')-C(23')-H(23')	119.9
C(22')-C(23')-H(23')	119.9
C(23')-C(24')-C(20')	121.26(16)
C(23')-C(24')-H(24')	119.4
C(20')-C(24')-H(24')	119.4
C(26')-C(25')-C(20')	120.66(19)
C(26')-C(25')-H(25')	119.7
C(20')-C(25')-H(25')	119.7
C(25')-C(26')-C(27')	120.47(18)
C(25')-C(26')-H(26')	119.8
C(27')-C(26')-H(26')	119.8
C(28')-C(27')-C(26')	120.8(2)
C(28')-C(27')-H(27')	119.6
C(26')-C(27')-H(27')	119.6
C(27')-C(28')-C(29')	120.25(18)
C(27')-C(28')-H(28')	119.9
C(29')-C(28')-H(28')	119.9
C(28')-C(29')-C(21')	122.06(15)
C(28')-C(29')-C(20')	118.66(16)
C(21')-C(29')-C(20')	119.24(16)
C(24')-C(20')-C(25')	121.88(17)
C(24')-C(20')-C(29')	118.93(16)
C(25')-C(20')-C(29')	119.14(19)
C(211)-N(2)-C(28)	123.98(17)
C(211)-N(2)-H(2)	114.4(15)
C(28)-N(2)-H(2)	120.8(15)
C(22')-O(2')-H(2')	108.4(18)

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for **32b**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(11)	36(1)	32(1)	24(1)	0(1)	0(1)	0(1)
C(12)	36(1)	42(1)	34(1)	-1(1)	-1(1)	-1(1)
C(13)	49(1)	39(1)	42(1)	-5(1)	-6(1)	-11(1)
C(14)	56(1)	30(1)	38(1)	-6(1)	-6(1)	0(1)
C(15)	53(1)	38(1)	40(1)	-7(1)	0(1)	12(1)
C(16)	46(1)	51(1)	46(1)	-2(1)	8(1)	13(1)
C(17)	37(1)	50(1)	44(1)	-4(1)	3(1)	-2(1)
C(18)	39(1)	37(1)	30(1)	-4(1)	3(1)	-2(1)
C(19)	38(1)	30(1)	25(1)	0(1)	0(1)	1(1)
C(110)	47(1)	32(1)	30(1)	-2(1)	-1(1)	5(1)
C(111)	39(1)	48(1)	67(1)	-23(1)	19(1)	-9(1)
C(112)	59(1)	64(1)	98(2)	-48(1)	28(1)	-20(1)
N(1)	39(1)	49(1)	40(1)	-17(1)	12(1)	-11(1)
O(1)	87(1)	45(1)	83(1)	-15(1)	47(1)	-12(1)
O(1')	118(1)	42(1)	27(1)	6(1)	-6(1)	-1(1)
C(11')	33(1)	32(1)	27(1)	1(1)	-1(1)	2(1)
C(12')	59(1)	35(1)	29(1)	3(1)	-6(1)	2(1)
C(13')	78(1)	33(1)	47(1)	6(1)	-13(1)	9(1)
C(14')	62(1)	36(1)	53(1)	-6(1)	-4(1)	13(1)
C(15')	51(1)	56(1)	42(1)	-18(1)	3(1)	5(1)
C(16')	58(1)	74(1)	29(1)	-9(1)	4(1)	-2(1)
C(17')	59(1)	64(1)	31(1)	7(1)	1(1)	4(1)
C(18')	44(1)	43(1)	29(1)	2(1)	0(1)	6(1)
C(19')	28(1)	36(1)	30(1)	-2(1)	-1(1)	3(1)
C(10')	38(1)	41(1)	38(1)	-6(1)	0(1)	7(1)
C(21)	32(1)	42(1)	28(1)	2(1)	-1(1)	-4(1)
C(22)	49(1)	53(1)	46(1)	-7(1)	1(1)	-17(1)
C(23)	53(1)	79(2)	60(1)	0(1)	-3(1)	-31(1)
C(24)	34(1)	98(2)	58(1)	15(1)	1(1)	-20(1)
C(25)	49(1)	96(2)	66(1)	24(1)	20(1)	30(1)
C(26)	84(2)	76(2)	79(2)	12(1)	33(2)	42(2)
C(27)	86(2)	44(1)	71(2)	6(1)	17(1)	22(1)
C(28)	49(1)	37(1)	40(1)	9(1)	2(1)	11(1)
C(29)	32(1)	46(1)	29(1)	10(1)	0(1)	5(1)
C(210)	35(1)	71(1)	41(1)	16(1)	4(1)	10(1)
C(211)	66(1)	29(1)	45(1)	-2(1)	7(1)	-1(1)
C(212)	79(2)	36(1)	101(2)	0(1)	22(2)	-14(1)
C(21')	33(1)	28(1)	33(1)	-2(1)	2(1)	-1(1)
C(22')	35(1)	32(1)	41(1)	4(1)	2(1)	0(1)
C(23')	32(1)	41(1)	61(1)	9(1)	-1(1)	6(1)
C(24')	33(1)	46(1)	69(1)	6(1)	14(1)	4(1)
C(25')	63(1)	49(1)	52(1)	-8(1)	28(1)	-4(1)
C(26')	88(2)	56(1)	34(1)	-7(1)	19(1)	-19(1)
C(27')	79(1)	52(1)	33(1)	-2(1)	-6(1)	-15(1)
C(28')	53(1)	40(1)	32(1)	-4(1)	-2(1)	-9(1)
C(29')	40(1)	26(1)	34(1)	-6(1)	6(1)	-2(1)
C(20')	44(1)	32(1)	48(1)	-5(1)	15(1)	0(1)
N(2)	48(1)	31(1)	51(1)	4(1)	-2(1)	4(1)
O(2)	81(1)	49(1)	44(1)	14(1)	4(1)	11(1)
O(2')	40(1)	58(1)	39(1)	13(1)	-6(1)	-4(1)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **32b**.

	x	y	z	U(eq)
H(12)	13537	1087	5046	45
H(13)	13349	2563	5608	52
H(14)	11844	3066	5982	50
H(15)	10107	2811	6116	52
H(16)	8747	1931	5895	57
H(17)	8847	552	5175	52
H(11A)	10211	-2499	4467	110
H(11B)	10636	-1760	3891	110
H(11C)	9513	-1947	3919	110
H(13')	12908	-2405	5251	63
H(14')	13098	-2640	3982	60
H(15')	13063	-2008	2652	60
H(16')	12766	-797	1833	64
H(17')	12273	664	2294	61
H(18')	12107	919	3570	46
H(22)	8125	1704	2928	59
H(23)	9696	2012	2528	77
H(24)	10555	894	1896	76
H(25)	10687	-707	1352	84
H(26)	10014	-2119	1046	96
H(27)	8460	-2502	1472	81
H(21A)	5952	-3040	3012	108
H(21B)	5681	-2009	2761	108
H(21C)	6022	-2207	3598	108
H(23')	4812	483	2020	54
H(24')	4329	112	3223	59
H(25')	4729	-355	4554	66
H(26')	5865	-728	5452	71
H(27')	7511	-648	5168	65
H(28')	8030	-186	3979	50
H(1)	10642(16)	-227(16)	4196(14)	57(6)
H(1')	12550(20)	-1400(20)	6236(16)	86(9)
H(2)	6760(17)	-1298(16)	2143(13)	53(6)
H(2')	6080(20)	788(19)	1233(15)	76(8)

Table S16. Torsion angles [deg] for **32b**.

C(19)-C(11)-C(12)-C(13)	2.4(2)
C(11')-C(11)-C(12)-C(13)	-175.36(14)
C(11)-C(12)-C(13)-C(14)	1.1(3)
C(12)-C(13)-C(14)-C(110)	-1.6(3)
C(110)-C(15)-C(16)-C(17)	-2.5(3)
C(15)-C(16)-C(17)-C(18)	3.3(3)
C(16)-C(17)-C(18)-N(1)	-176.66(17)
C(16)-C(17)-C(18)-C(19)	0.6(3)
C(17)-C(18)-C(19)-C(110)	-4.9(2)
N(1)-C(18)-C(19)-C(110)	172.35(15)
C(17)-C(18)-C(19)-C(11)	175.77(17)
N(1)-C(18)-C(19)-C(11)	-7.0(2)
C(12)-C(11)-C(19)-C(18)	174.19(16)
C(11')-C(11)-C(19)-C(18)	-8.2(2)
C(12)-C(11)-C(19)-C(110)	-5.2(2)
C(11')-C(11)-C(19)-C(110)	172.38(14)
C(13)-C(14)-C(110)-C(15)	178.44(18)
C(13)-C(14)-C(110)-C(19)	-1.4(3)
C(16)-C(15)-C(110)-C(14)	178.23(18)
C(16)-C(15)-C(110)-C(19)	-2.0(3)
C(18)-C(19)-C(110)-C(14)	-174.70(16)
C(11)-C(19)-C(110)-C(14)	4.7(2)
C(18)-C(19)-C(110)-C(15)	5.5(2)
C(11)-C(19)-C(110)-C(15)	-175.08(15)
O(1)-C(111)-N(1)-C(18)	2.2(3)
C(112)-C(111)-N(1)-C(18)	-178.90(19)
C(17)-C(18)-N(1)-C(111)	-61.9(3)
C(19)-C(18)-N(1)-C(111)	120.8(2)
C(12)-C(11)-C(11')-C(12')	89.5(2)
C(19)-C(11)-C(11')-C(12')	-88.1(2)
C(12)-C(11)-C(11')-C(19')	-86.29(19)
C(19)-C(11)-C(11')-C(19')	96.10(19)
C(19')-C(11')-C(12')-O(1')	179.92(16)
C(11)-C(11')-C(12')-O(1')	4.0(3)
C(19')-C(11')-C(12')-C(13')	-0.2(3)
C(11)-C(11')-C(12')-C(13')	-176.13(18)
O(1')-C(12')-C(13')-C(14')	-179.7(2)
C(11')-C(12')-C(13')-C(14')	0.4(3)
C(12')-C(13')-C(14')-C(10')	-0.6(3)
C(10')-C(15')-C(16')-C(17')	0.4(3)
C(15')-C(16')-C(17')-C(18')	0.8(3)
C(16')-C(17')-C(18')-C(19')	-0.4(3)
C(17')-C(18')-C(19')-C(11')	-179.48(17)
C(17')-C(18')-C(19')-C(10')	-1.2(3)
C(12')-C(11')-C(19')-C(18')	178.46(16)
C(11)-C(11')-C(19')-C(18')	-5.6(2)
C(12')-C(11')-C(19')-C(10')	0.2(2)
C(11)-C(11')-C(19')-C(10')	176.11(15)
C(13')-C(14')-C(10')-C(15')	179.5(2)
C(13')-C(14')-C(10')-C(19')	0.6(3)
C(16')-C(15')-C(10')-C(14')	179.1(2)
C(16')-C(15')-C(10')-C(19')	-2.0(3)
C(18')-C(19')-C(10')-C(14')	-178.73(17)
C(11')-C(19')-C(10')-C(14')	-0.4(3)
C(18')-C(19')-C(10')-C(15')	2.3(2)
C(11')-C(19')-C(10')-C(15')	-179.32(16)
C(29)-C(21)-C(22)-C(23)	1.2(3)
C(21')-C(21)-C(22)-C(23)	-174.30(18)
C(21)-C(22)-C(23)-C(24)	0.2(3)
C(22)-C(23)-C(24)-C(210)	-1.1(3)

C(210)-C(25)-C(26)-C(27)	-2.5(4)
C(25)-C(26)-C(27)-C(28)	0.7(4)
C(26)-C(27)-C(28)-N(2)	-177.1(2)
C(26)-C(27)-C(28)-C(29)	2.9(3)
C(27)-C(28)-C(29)-C(210)	-4.4(3)
N(2)-C(28)-C(29)-C(210)	175.61(16)
C(27)-C(28)-C(29)-C(21)	174.82(18)
N(2)-C(28)-C(29)-C(21)	-5.2(3)
C(22)-C(21)-C(29)-C(28)	179.27(17)
C(21')-C(21)-C(29)-C(28)	-5.5(2)
C(22)-C(21)-C(29)-C(210)	-1.6(2)
C(21')-C(21)-C(29)-C(210)	173.62(15)
C(26)-C(25)-C(210)-C(24)	-176.5(2)
C(26)-C(25)-C(210)-C(29)	0.9(3)
C(23)-C(24)-C(210)-C(25)	178.0(2)
C(23)-C(24)-C(210)-C(29)	0.6(3)
C(28)-C(29)-C(210)-C(25)	2.5(3)
C(21)-C(29)-C(210)-C(25)	-176.71(17)
C(28)-C(29)-C(210)-C(24)	179.96(17)
C(21)-C(29)-C(210)-C(24)	0.7(2)
C(22)-C(21)-C(21')-C(22')	93.24(19)
C(29)-C(21)-C(21')-C(22')	-82.0(2)
C(22)-C(21)-C(21')-C(29')	-87.29(19)
C(29)-C(21)-C(21')-C(29')	97.45(18)
C(29')-C(21')-C(22')-O(2')	-177.02(14)
C(21)-C(21')-C(22')-O(2')	2.5(2)
C(29')-C(21')-C(22')-C(23')	-0.1(2)
C(21)-C(21')-C(22')-C(23')	179.38(15)
O(2')-C(22')-C(23')-C(24')	178.41(17)
C(21')-C(22')-C(23')-C(24')	1.6(3)
C(22')-C(23')-C(24')-C(20')	-1.6(3)
C(20')-C(25')-C(26')-C(27')	0.1(3)
C(25')-C(26')-C(27')-C(28')	0.2(3)
C(26')-C(27')-C(28')-C(29')	0.0(3)
C(27')-C(28')-C(29')-C(21')	-178.24(16)
C(27')-C(28')-C(29')-C(20')	-0.6(2)
C(22')-C(21')-C(29')-C(28')	176.32(15)
C(21)-C(21')-C(29')-C(28')	-3.1(2)
C(22')-C(21')-C(29')-C(20')	-1.3(2)
C(21)-C(21')-C(29')-C(20')	179.22(15)
C(23')-C(24')-C(20')-C(25')	-177.10(18)
C(23')-C(24')-C(20')-C(29')	0.2(3)
C(26')-C(25')-C(20')-C(24')	176.58(19)
C(26')-C(25')-C(20')-C(29')	-0.7(3)
C(28')-C(29')-C(20')-C(24')	-176.44(16)
C(21')-C(29')-C(20')-C(24')	1.3(2)
C(28')-C(29')-C(20')-C(25')	0.9(2)
C(21')-C(29')-C(20')-C(25')	178.65(16)
O(2)-C(211)-N(2)-C(28)	-3.6(3)
C(212)-C(211)-N(2)-C(28)	176.15(18)
C(27)-C(28)-N(2)-C(211)	72.1(2)
C(29)-C(28)-N(2)-C(211)	-107.83(19)

Symmetry transformations used to generate equivalent atoms:

Table S17. Hydrogen bonds for **32b** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1')-H(1')...O(2)#1	0.90(3)	1.81(3)	2.7030(19)	175(3)
O(2')-H(2')...O(1)#2	0.85(3)	1.85(3)	2.6535(19)	157(3)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y-1/2,-z+1 #2 -x+3/2,-y,z-1/2

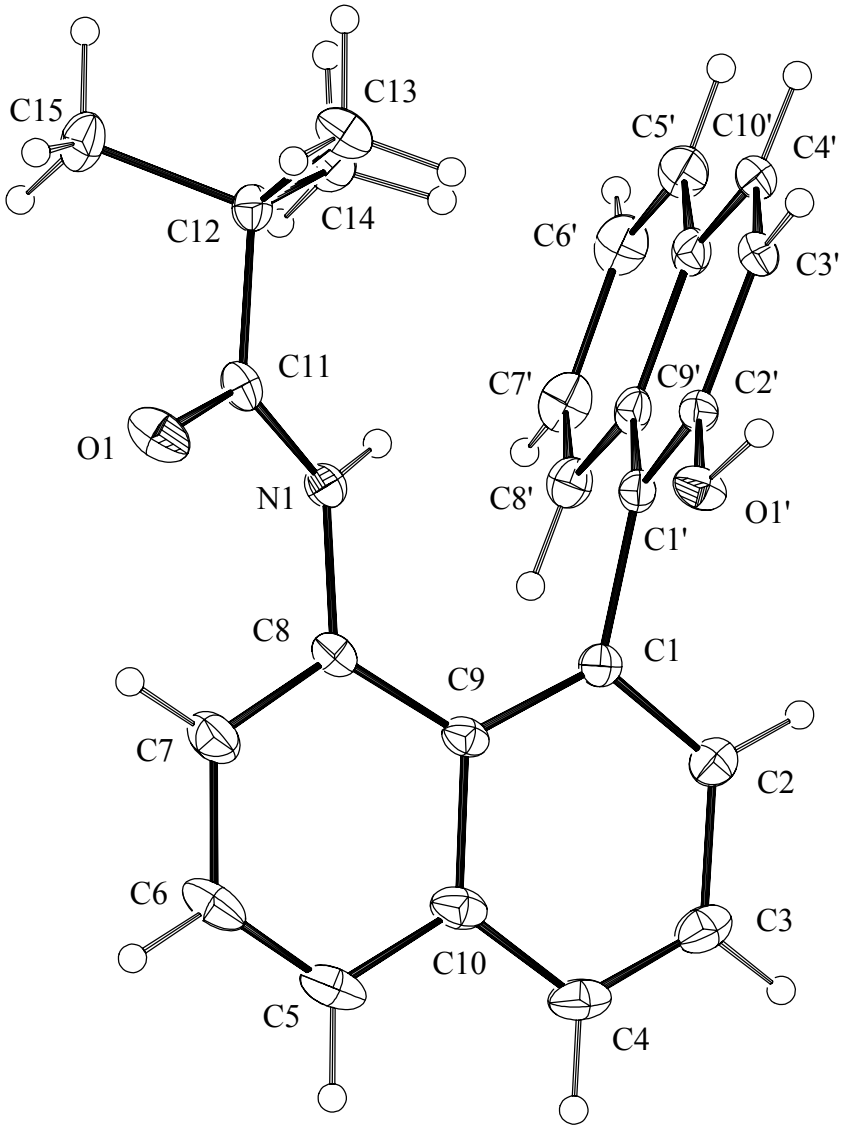

Figure S25. An ORTEP diagram of **32d**. The thermal ellipsoids are drawn on 30% probability level.

Table S18. Crystal data and structure refinement for **32d**.

Identification code	**32d**
Empirical formula	C25 H23 N O2
Formula weight	369.44
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 7.7500(2) A alpha = 90 deg. b = 9.6320(2) A beta = 102.5610(15) deg. c = 13.4030(3) A gamma = 90 deg.
Volume	976.56(4) A^3
Z, Calculated density	2, 1.256 Mg/m^3
Absorption coefficient	0.079 mm^-1
F(000)	392
Crystal size	0.5 x 0.3 x 0.17 mm
Theta range for data collection	3.42 to 27.51 deg.
Limiting indices	-10<=h<=10, -12<=k<=12, -17<=l<=17
Reflections collected / unique	15820 / 4446 [R(int) = 0.0300]
Completeness to theta = 27.51	99.2 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4446 / 1 / 264
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0351, wR2 = 0.0861
R indices (all data)	R1 = 0.0384, wR2 = 0.0885
Absolute structure parameter	-0.6(9)
Largest diff. peak and hole	0.327 and -0.153 e.A^-3

Table S19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **32d**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2493(2)	6462(1)	6936(1)	22(1)
C(2)	1033(2)	5789(2)	6364(1)	28(1)
C(3)	-477(2)	6504(2)	5843(1)	34(1)
C(4)	-530(2)	7903(2)	5904(1)	34(1)
C(5)	789(2)	10128(2)	6529(1)	38(1)
C(6)	2151(2)	10891(2)	7047(1)	44(1)
C(7)	3732(2)	10238(2)	7540(1)	37(1)
C(8)	3915(2)	8819(1)	7526(1)	26(1)
C(9)	2491(2)	7953(1)	6997(1)	23(1)
C(10)	919(2)	8665(2)	6474(1)	30(1)
N(1)	5563(2)	8206(1)	7997(1)	25(1)
O(1)	6704(2)	9903(1)	9118(1)	36(1)
C(11)	6845(2)	8749(1)	8743(1)	23(1)
C(12)	8505(2)	7877(1)	9128(1)	24(1)
C(13)	8644(2)	6609(1)	8469(1)	27(1)
C(14)	8472(2)	7431(2)	10226(1)	34(1)
C(15)	10111(2)	8813(2)	9148(1)	37(1)
O(1')	3197(1)	6000(1)	9037(1)	28(1)
C(1')	3929(2)	5499(1)	7462(1)	21(1)
C(2')	4131(2)	5218(1)	8494(1)	22(1)
C(3')	5281(2)	4150(1)	8975(1)	25(1)
C(4')	6219(2)	3379(1)	8424(1)	28(1)
C(5')	7110(2)	2874(2)	6797(1)	34(1)
C(6')	6977(2)	3132(2)	5782(1)	37(1)
C(7')	5811(2)	4163(2)	5289(1)	34(1)
C(8')	4824(2)	4933(2)	5822(1)	28(1)
C(9')	4929(2)	4700(1)	6879(1)	23(1)
C(10')	6098(2)	3640(1)	7372(1)	25(1)

Table S20. Bond lengths [A] and angles [deg] for **32d**.

C(1)-C(2)	1.3829(19)
C(1)-C(9)	1.4389(18)
C(1)-C(1')	1.5017(17)
C(2)-C(3)	1.405(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.351(2)
C(3)-H(3)	0.9300
C(4)-C(10)	1.418(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.348(3)
C(5)-C(10)	1.415(2)
C(5)-H(5)	0.9300
C(6)-C(7)	1.408(2)
C(6)-H(6)	0.9300
C(7)-C(8)	1.375(2)
C(7)-H(7)	0.9300
C(8)-N(1)	1.4242(17)
C(8)-C(9)	1.440(2)
C(9)-C(10)	1.4407(18)
N(1)-C(11)	1.3516(18)
N(1)-H(1)	0.812(19)
O(1)-C(11)	1.2355(16)
C(11)-C(12)	1.5292(18)
C(12)-C(13)	1.5255(18)
C*(12)-C(15)	1.5324(19)
C(12)-C(14)	1.5386(19)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
O(1')-C(2')	1.3593(15)
O(1')-H(1')	0.86(2)
C(1')-C(2')	1.3846(18)
C(1')-C(9')	1.4372(18)
C(2')-C(3')	1.4205(18)
C(3')-C(4')	1.364(2)
C(3')-H(3')	0.9300
C(4')-C(10')	1.414(2)
C(4')-H(4')	0.9300
C(5')-C(6')	1.364(2)
C(5')-C(10')	1.4211(19)
C(5')-H(5')	0.9300
C(6')-C(7')	1.407(2)
C(6')-H(6')	0.9300
C(7')-C(8')	1.372(2)
C(7')-H(7')	0.9300
C(8')-C(9')	1.4194(19)
C(8')-H(8')	0.9300
C(9')-C(10')	1.4284(18)
C(2)-C(1)-C(9)	119.26(12)
C(2)-C(1)-C(1')	113.86(12)
C(9)-C(1)-C(1')	126.85(12)
C(1)-C(2)-C(3)	122.55(14)
C(1)-C(2)-H(2)	118.7

C(3)-C(2)-H(2)	118.7
C(4)-C(3)-C(2)	119.50(15)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(10)	121.17(14)
C(3)-C(4)-H(4)	119.4
C(10)-C(4)-H(4)	119.4
C(6)-C(5)-C(10)	120.89(14)
C(6)-C(5)-H(5)	119.6
C(10)-C(5)-H(5)	119.6
C(5)-C(6)-C(7)	120.12(15)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	121.31(15)
C(8)-C(7)-H(7)	119.3
C(6)-C(7)-H(7)	119.3
C(7)-C(8)-N(1)	119.42(13)
C(7)-C(8)-C(9)	120.82(13)
N(1)-C(8)-C(9)	119.68(12)
C(1)-C(9)-C(8)	126.59(12)
C(1)-C(9)-C(10)	117.31(13)
C(8)-C(9)-C(10)	116.10(12)
C(5)-C(10)-C(4)	119.11(14)
C(5)-C(10)-C(9)	120.69(14)
C(4)-C(10)-C(9)	120.19(13)
C(11)-N(1)-C(8)	127.73(12)
C(11)-N(1)-H(1)	115.6(12)
C(8)-N(1)-H(1)	116.6(12)
O(1)-C(11)-N(1)	122.24(13)
O(1)-C(11)-C(12)	119.91(12)
N(1)-C(11)-C(12)	117.85(11)
C(13)-C(12)-C(11)	113.80(11)
C(13)-C(12)-C(15)	108.77(12)
C(11)-C(12)-C(15)	107.67(11)
C(13)-C(12)-C(14)	110.42(11)
C(11)-C(12)-C(14)	106.78(11)
C(15)-C(12)-C(14)	109.29(11)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(2')-O(1')-H(1')	106.3(14)
C(2')-C(1')-C(9')	118.81(11)
C(2')-C(1')-C(1)	120.05(11)
C(9')-C(1')-C(1)	120.48(11)
O(1')-C(2')-C(1')	117.99(11)
O(1')-C(2')-C(3')	120.86(11)
C(1')-C(2')-C(3')	121.14(11)
C(4')-C(3')-C(2')	120.34(12)
C(4')-C(3')-H(3')	119.8

C(2')-C(3')-H(3')	119.8
C(3')-C(4')-C(10')	121.00(12)
C(3')-C(4')-H(4')	119.5
C(10')-C(4')-H(4')	119.5
C(6')-C(5')-C(10')	121.07(14)
C(6')-C(5')-H(5')	119.5
C(10')-C(5')-H(5')	119.5
C(5')-C(6')-C(7')	119.85(14)
C(5')-C(6')-H(6')	120.1
C(7')-C(6')-H(6')	120.1
C(8')-C(7')-C(6')	120.75(14)
C(8')-C(7')-H(7')	119.6
C(6')-C(7')-H(7')	119.6
C(7')-C(8')-C(9')	121.13(14)
C(7')-C(8')-H(8')	119.4
C(9')-C(8')-H(8')	119.4
C(8')-C(9')-C(10')	117.89(12)
C(8')-C(9')-C(1')	122.52(12)
C(10')-C(9')-C(1')	119.58(11)
C(4')-C(10')-C(5')	121.61(12)
C(4')-C(10')-C(9')	119.10(11)
C(5')-C(10')-C(9')	119.29(12)

Symmetry transformations used to generate equivalent atoms:

Table S21. Anisotropic displacement parameters (A^2 x 10^3) for **32d**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	22(1)	26(1)	20(1)	2(1)	7(1)	1(1)
C(2)	27(1)	32(1)	26(1)	-1(1)	6(1)	-2(1)
C(3)	24(1)	51(1)	27(1)	1(1)	2(1)	-2(1)
C(4)	26(1)	53(1)	24(1)	7(1)	4(1)	11(1)
C(5)	44(1)	39(1)	32(1)	11(1)	8(1)	20(1)
C(6)	57(1)	26(1)	46(1)	8(1)	7(1)	16(1)
C(7)	45(1)	23(1)	40(1)	3(1)	2(1)	3(1)
C(8)	30(1)	22(1)	25(1)	5(1)	6(1)	3(1)
C(9)	25(1)	26(1)	19(1)	5(1)	7(1)	6(1)
C(10)	30(1)	38(1)	23(1)	7(1)	9(1)	11(1)
N(1)	27(1)	16(1)	31(1)	-2(1)	5(1)	1(1)
O(1)	56(1)	24(1)	25(1)	-6(1)	3(1)	10(1)
C(11)	33(1)	19(1)	18(1)	0(1)	9(1)	-1(1)
C(12)	26(1)	22(1)	24(1)	-2(1)	5(1)	-3(1)
C(13)	24(1)	24(1)	34(1)	-7(1)	7(1)	0(1)
C(14)	44(1)	30(1)	27(1)	4(1)	8(1)	8(1)
C(15)	35(1)	31(1)	44(1)	-7(1)	7(1)	-12(1)
O(1')	31(1)	32(1)	23(1)	6(1)	11(1)	10(1)
C(1')	21(1)	18(1)	24(1)	0(1)	6(1)	-3(1)
C(2')	21(1)	20(1)	26(1)	1(1)	7(1)	0(1)
C(3')	26(1)	22(1)	27(1)	6(1)	6(1)	0(1)
C(4')	25(1)	18(1)	38(1)	3(1)	5(1)	1(1)
C(5')	32(1)	22(1)	49(1)	-7(1)	13(1)	3(1)
C(6')	36(1)	32(1)	46(1)	-13(1)	18(1)	-1(1)
C(7')	36(1)	39(1)	31(1)	-9(1)	14(1)	-4(1)
C(8')	29(1)	27(1)	28(1)	-4(1)	7(1)	-3(1)
C(9')	23(1)	18(1)	29(1)	-4(1)	7(1)	-5(1)
C(10')	25(1)	17(1)	34(1)	-4(1)	8(1)	-3(1)

Table S22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **32d**.

	x	y	z	U(eq)
H(2)	1050	4825	6322	34
H(3)	-1431	6018	5460	41
H(4)	-1536	8375	5566	41
H(5)	-249	10568	6204	46
H(6)	2046	11851	7078	52
H(7)	4671	10777	7882	45
H(13A)	8557	6896	7774	41
H(13B)	7702	5975	8501	41
H(13C)	9760	6158	8716	41
H(14A)	7487	6823	10214	50
H(14B)	8358	8237	10628	50
H(14C)	9550	6955	10522	50
H(15A)	11174	8274	9338	55
H(15B)	10127	9544	9637	55
H(15C)	10039	9207	8482	55
H(3')	5395	3976	9668	30
H(4')	6951	2671	8744	33
H(5')	7876	2185	7117	41
H(6')	7656	2627	5417	44
H(7')	5707	4325	4595	41
H(8')	4074	5619	5485	33
H(1)	5760(20)	7440(20)	7802(12)	26(4)
H(1')	3280(30)	5590(20)	9613(17)	49(6)

Table S23. Torsion angles [deg] for **32d**.

C(9)-C(1)-C(2)-C(3)	-0.7(2)
C(1')-C(1)-C(2)-C(3)	177.68(12)
C(1)-C(2)-C(3)-C(4)	-0.6(2)
C(2)-C(3)-C(4)-C(10)	0.8(2)
C(10)-C(5)-C(6)-C(7)	0.2(3)
C(5)-C(6)-C(7)-C(8)	-1.4(3)
C(6)-C(7)-C(8)-N(1)	177.30(14)
C(6)-C(7)-C(8)-C(9)	0.4(2)
C(2)-C(1)-C(9)-C(8)	-177.71(12)
C(1')-C(1)-C(9)-C(8)	4.1(2)
C(2)-C(1)-C(9)-C(10)	1.80(18)
C(1')-C(1)-C(9)-C(10)	-176.35(11)
C(7)-C(8)-C(9)-C(1)	-178.88(14)
N(1)-C(8)-C(9)-C(1)	4.2(2)
C(7)-C(8)-C(9)-C(10)	1.61(19)
N(1)-C(8)-C(9)-C(10)	-175.27(11)
C(6)-C(5)-C(10)-C(4)	-178.70(15)
C(6)-C(5)-C(10)-C(9)	1.9(2)
C(3)-C(4)-C(10)-C(5)	-178.95(15)
C(3)-C(4)-C(10)-C(9)	0.4(2)
C(1)-C(9)-C(10)-C(5)	177.67(14)
C(8)-C(9)-C(10)-C(5)	-2.77(18)
C(1)-C(9)-C(10)-C(4)	-1.68(18)
C(8)-C(9)-C(10)-C(4)	177.88(12)
C(7)-C(8)-N(1)-C(11)	23.1(2)
C(9)-C(8)-N(1)-C(11)	-159.96(12)
C(8)-N(1)-C(11)-O(1)	0.3(2)
C(8)-N(1)-C(11)-C(12)	179.74(12)
O(1)-C(11)-C(12)-C(13)	-169.37(12)
N(1)-C(11)-C(12)-C(13)	11.19(17)
O(1)-C(11)-C(12)-C(15)	-48.73(16)
N(1)-C(11)-C(12)-C(15)	131.83(13)
O(1)-C(11)-C(12)-C(14)	68.54(16)
N(1)-C(11)-C(12)-C(14)	-110.90(13)
C(2)-C(1)-C(1')-C(2')	-101.71(14)
C(9)-C(1)-C(1')-C(2')	76.53(17)
C(2)-C(1)-C(1')-C(9')	68.82(15)
C(9)-C(1)-C(1')-C(9')	-112.94(15)
C(9')-C(1')-C(2')-O(1')	178.92(11)
C(1)-C(1')-C(2')-O(1')	-10.39(18)
C(9')-C(1')-C(2')-C(3')	-0.86(18)
C(1)-C(1')-C(2')-C(3')	169.82(12)
O(1')-C(2')-C(3')-C(4')	-179.56(12)
C(1')-C(2')-C(3')-C(4')	0.21(19)
C(2')-C(3')-C(4')-C(10')	1.2(2)
C(10')-C(5')-C(6')-C(7')	-0.5(2)
C(5')-C(6')-C(7')-C(8')	1.2(2)
C(6')-C(7')-C(8')-C(9')	-1.0(2)
C(7')-C(8')-C(9')-C(10')	0.15(19)
C(7')-C(8')-C(9')-C(1')	179.24(13)
C(2')-C(1')-C(9')-C(8')	-178.97(12)
C(1)-C(1')-C(9')-C(8')	10.38(18)
C(2')-C(1')-C(9')-C(10')	0.10(17)
C(1)-C(1')-C(9')-C(10')	-170.55(11)
C(3')-C(4')-C(10')-C(5')	177.97(13)
C(3')-C(4')-C(10')-C(9')	-1.96(19)
C(6')-C(5')-C(10')-C(4')	179.80(14)
C(6')-C(5')-C(10')-C(9')	-0.3(2)
C(8')-C(9')-C(10')-C(4')	-179.60(12)
C(1')-C(9')-C(10')-C(4')	1.28(17)

C(8')-C(9')-C(10')-C(5')	0.46(18)
C(1')-C(9')-C(10')-C(5')	-178.66(12)

Symmetry transformations used to generate equivalent atoms:

Table S24. Hydrogen bonds for **32d** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1')-H(1')...O(1)#1	0.86(2)	1.82(2)	2.6741(14)	173(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+2

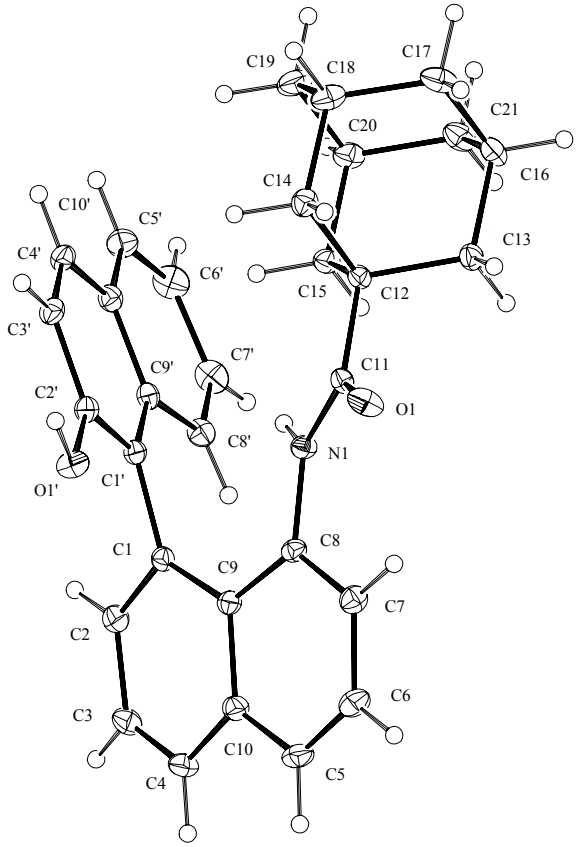

Figure S26. An ORTEP diagram of **32f**. The thermal ellipsoids are drawn on 30% probability level.

Table S25. Crystal data and structure refinement for **32f**.

Identification code	**32f**
Empirical formula	C31 H29 N O2
Formula weight	447.55
Temperature	150(2) K
Wavelength	0.71070 A
Crystal system, space group	Monoclinic, P 21
Unit cell dimensions	a = 11.1730(2) A alpha = 90 deg. b = 8.9400(2) A beta = 98.0110(12) deg. c = 11.6690(2) A gamma = 90 deg.
Volume	1154.20(4) A^3
Z, Calculated density	2, 1.288 Mg/m^3
Absorption coefficient	0.080 mm^-1
F(000)	476
Crystal size	0.25 x 0.25 x 0.12 mm
Theta range for data collection	3.53 to 27.48 deg.
Limiting indices	-14<=h<=14, -10<=k<=11, -15<=l<=15
Reflections collected / unique	17572 / 5180 [R(int) = 0.0270]
Completeness to theta = 27.48	99.6 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5180 / 1 / 315
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0333, wR2 = 0.0788
R indices (all data)	R1 = 0.0366, wR2 = 0.0813
Absolute structure parameter	0.1(8)
Largest diff. peak and hole	0.171 and -0.167 e.A^-3

Table S26. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **32f**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(1)	7995(1)	2191(1)	4671(1)	20(1)
O(1')	7805(1)	5729(1)	4882(1)	25(1)
O(1)	9965(1)	1654(1)	5270(1)	29(1)
C(1)	5766(1)	3943(1)	4824(1)	19(1)
C(2)	4622(1)	4455(2)	4921(1)	25(1)
C(3)	4076(1)	4233(2)	5921(1)	29(1)
C(4)	4701(1)	3538(2)	6852(1)	28(1)
C(5)	6477(1)	2165(2)	7772(1)	27(1)
C(6)	7556(1)	1498(2)	7721(1)	28(1)
C(7)	8084(1)	1555(2)	6694(1)	25(1)
C(8)	7532(1)	2314(1)	5742(1)	19(1)
C(9)	6416(1)	3096(1)	5765(1)	19(1)
C(10)	5872(1)	2953(2)	6804(1)	23(1)
C(11)	9115(1)	1801(1)	4476(1)	20(1)
C(12)	9292(1)	1499(1)	3222(1)	18(1)
C(13)	9686(1)	-155(1)	3154(1)	22(1)
C(14)	10305(1)	2522(2)	2901(1)	24(1)
C(15)	8158(1)	1738(2)	2333(1)	21(1)
C(16)	9953(1)	-511(2)	1930(1)	27(1)
C(17)	10973(1)	504(2)	1649(1)	33(1)
C(18)	10576(1)	2139(2)	1682(1)	31(1)
C(19)	9436(1)	2392(2)	808(1)	33(1)
C(20)	8424(1)	1375(2)	1108(1)	26(1)
C(21)	8813(1)	-258(2)	1054(1)	29(1)
C(1')	6252(1)	4405(1)	3741(1)	18(1)
C(2')	7244(1)	5347(1)	3814(1)	20(1)
C(3')	7666(1)	5903(2)	2806(1)	22(1)
C(4')	7067(1)	5560(2)	1738(1)	22(1)
C(5')	5416(1)	4255(2)	505(1)	29(1)
C(6')	4444(1)	3310(2)	391(1)	34(1)
C(7')	4071(1)	2666(2)	1381(1)	32(1)
C(8')	4642(1)	3003(2)	2466(1)	25(1)
C(9')	5633(1)	4017(1)	2622(1)	20(1)
C(10')	6036(1)	4620(1)	1609(1)	21(1)

Table S27. Bond lengths [A] and angles [deg] for **32f**.

N(1)-C(11)	1.3480(16)
N(1)-C(8)	1.4217(15)
N(1)-H(1)	0.879(16)
O(1')-C(2')	1.3577(15)
O(1')-H(1')	0.98(2)
O(1)-C(11)	1.2375(15)
C(1)-C(2)	1.3774(18)
C(1)-C(9)	1.4435(18)
C(1)-C(1')	1.5013(17)
C(2)-C(3)	1.4036(19)
C(2)-H(2)	0.9300
C(3)-C(4)	1.358(2)
C(3)-H(3)	0.9300
C(4)-C(10)	1.417(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.354(2)
C(5)-C(10)	1.4193(19)
C(5)-H(5)	0.9300
C(6)-C(7)	1.4074(18)
C(6)-H(6)	0.9300
C(7)-C(8)	1.3730(17)
C(7)-H(7)	0.9300
C(8)-C(9)	1.4332(17)
C(9)-C(10)	1.4367(17)
C(11)-C(12)	1.5289(17)
C(12)-C(15)	1.5367(16)
C(12)-C(14)	1.5406(17)
C(12)-C(13)	1.5471(17)
C(13)-C(16)	1.5329(17)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(18)	1.5338(19)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(20)	1.5352(17)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(16)-C(17)	1.528(2)
C(16)-C(21)	1.5357(19)
C(16)-H(16)	0.9800
C(17)-C(18)	1.529(2)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.534(2)
C(18)-H(18)	0.9800
C(19)-C(20)	1.529(2)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(20)-C(21)	1.527(2)
C(20)-H(20)	0.9800
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(1')-C(2')	1.3859(17)
C(1')-C(9')	1.4319(17)
C(2')-C(3')	1.4172(18)
C(3')-C(4')	1.3647(18)
C(3')-H(3')	0.9300
C(4')-C(10')	1.4166(18)
C(4')-H(4')	0.9300
C(5')-C(6')	1.368(2)

C(5')-C(10')	1.4137(18)
C(5')-H(5')	0.9300
C(6')-C(7')	1.405(2)
C(6')-H(6')	0.9300
C(7')-C(8')	1.370(2)
C(7')-H(7')	0.9300
C(8')-C(9')	1.4229(18)
C(8')-H(8')	0.9300
C(9')-C(10')	1.4287(18)

C(11)-N(1)-C(8)	128.89(11)
C(11)-N(1)-H(1)	115.6(10)
C(8)-N(1)-H(1)	115.5(10)
C(2')-O(1')-H(1')	109.6(12)
C(2)-C(1)-C(9)	119.09(12)
C(2)-C(1)-C(1')	115.24(11)
C(9)-C(1)-C(1')	125.59(11)
C(1)-C(2)-C(3)	122.52(12)
C(1)-C(2)-H(2)	118.7
C(3)-C(2)-H(2)	118.7
C(4)-C(3)-C(2)	119.66(12)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(3)-C(4)-C(10)	120.83(13)
C(3)-C(4)-H(4)	119.6
C(10)-C(4)-H(4)	119.6
C(6)-C(5)-C(10)	120.78(12)
C(6)-C(5)-H(5)	119.6
C(10)-C(5)-H(5)	119.6
C(5)-C(6)-C(7)	120.19(12)
C(5)-C(6)-H(6)	119.9
C(7)-C(6)-H(6)	119.9
C(8)-C(7)-C(6)	120.85(12)
C(8)-C(7)-H(7)	119.6
C(6)-C(7)-H(7)	119.6
C(7)-C(8)-N(1)	119.75(11)
C(7)-C(8)-C(9)	121.29(11)
N(1)-C(8)-C(9)	118.58(10)
C(8)-C(9)-C(10)	116.37(11)
C(8)-C(9)-C(1)	126.06(11)
C(10)-C(9)-C(1)	117.49(11)
C(4)-C(10)-C(5)	119.47(12)
C(4)-C(10)-C(9)	120.12(12)
C(5)-C(10)-C(9)	120.34(12)
O(1)-C(11)-N(1)	122.35(11)
O(1)-C(11)-C(12)	120.60(11)
N(1)-C(11)-C(12)	117.02(10)
C(11)-C(12)-C(15)	114.59(10)
C(11)-C(12)-C(14)	108.98(10)
C(15)-C(12)-C(14)	108.55(10)
C(11)-C(12)-C(13)	107.05(10)
C(15)-C(12)-C(13)	108.22(10)
C(14)-C(12)-C(13)	109.36(10)
C(16)-C(13)-C(12)	109.84(10)
C(16)-C(13)-H(13A)	109.7
C(12)-C(13)-H(13A)	109.7
C(16)-C(13)-H(13B)	109.7
C(12)-C(13)-H(13B)	109.7
H(13A)-C(13)-H(13B)	108.2
C(18)-C(14)-C(12)	109.85(11)
C(18)-C(14)-H(14A)	109.7
C(12)-C(14)-H(14A)	109.7
C(18)-C(14)-H(14B)	109.7
C(12)-C(14)-H(14B)	109.7

H(14A)-C(14)-H(14B)	108.2
C(20)-C(15)-C(12)	110.46(10)
C(20)-C(15)-H(15A)	109.6
C(12)-C(15)-H(15A)	109.6
C(20)-C(15)-H(15B)	109.6
C(12)-C(15)-H(15B)	109.6
H(15A)-C(15)-H(15B)	108.1
C(17)-C(16)-C(13)	108.94(11)
C(17)-C(16)-C(21)	110.06(12)
C(13)-C(16)-C(21)	109.80(11)
C(17)-C(16)-H(16)	109.3
C(13)-C(16)-H(16)	109.3
C(21)-C(16)-H(16)	109.3
C(16)-C(17)-C(18)	109.58(11)
C(16)-C(17)-H(17A)	109.8
C(18)-C(17)-H(17A)	109.8
C(16)-C(17)-H(17B)	109.8
C(18)-C(17)-H(17B)	109.8
H(17A)-C(17)-H(17B)	108.2
C(17)-C(18)-C(14)	109.37(11)
C(17)-C(18)-C(19)	109.95(13)
C(14)-C(18)-C(19)	109.31(11)
C(17)-C(18)-H(18)	109.4
C(14)-C(18)-H(18)	109.4
C(19)-C(18)-H(18)	109.4
C(20)-C(19)-C(18)	109.38(12)
C(20)-C(19)-H(19A)	109.8
C(18)-C(19)-H(19A)	109.8
C(20)-C(19)-H(19B)	109.8
C(18)-C(19)-H(19B)	109.8
H(19A)-C(19)-H(19B)	108.2
C(21)-C(20)-C(19)	109.59(12)
C(21)-C(20)-C(15)	109.52(11)
C(19)-C(20)-C(15)	109.48(11)
C(21)-C(20)-H(20)	109.4
C(19)-C(20)-H(20)	109.4
C(15)-C(20)-H(20)	109.4
C(20)-C(21)-C(16)	109.14(11)
C(20)-C(21)-H(21A)	109.9
C(16)-C(21)-H(21A)	109.9
C(20)-C(21)-H(21B)	109.9
C(16)-C(21)-H(21B)	109.9
H(21A)-C(21)-H(21B)	108.3
C(2')-C(1')-C(9')	118.98(11)
C(2')-C(1')-C(1)	119.65(11)
C(9')-C(1')-C(1)	121.05(11)
O(1')-C(2')-C(1')	118.23(11)
O(1')-C(2')-C(3')	120.61(11)
C(1')-C(2')-C(3')	121.16(11)
C(4')-C(3')-C(2')	120.14(12)
C(4')-C(3')-H(3')	119.9
C(2')-C(3')-H(3')	119.9
C(3')-C(4')-C(10')	121.21(12)
C(3')-C(4')-H(4')	119.4
C(10')-C(4')-H(4')	119.4
C(6')-C(5')-C(10')	120.89(13)
C(6')-C(5')-H(5')	119.6
C(10')-C(5')-H(5')	119.6
C(5')-C(6')-C(7')	119.69(13)
C(5')-C(6')-H(6')	120.2
C(7')-C(6')-H(6')	120.2
C(8')-C(7')-C(6')	121.15(13)
C(8')-C(7')-H(7')	119.4
C(6')-C(7')-H(7')	119.4

C(7')-C(8')-C(9')	120.80(13)
C(7')-C(8')-H(8')	119.6
C(9')-C(8')-H(8')	119.6
C(8')-C(9')-C(10')	117.68(11)
C(8')-C(9')-C(1')	122.62(12)
C(10')-C(9')-C(1')	119.66(11)
C(5')-C(10')-C(4')	121.48(12)
C(5')-C(10')-C(9')	119.71(12)
C(4')-C(10')-C(9')	118.80(11)

Symmetry transformations used to generate equivalent atoms:

Table S28. Anisotropic displacement parameters (A^2 x 10^3) for **32f**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(1)	19(1)	23(1)	16(1)	2(1)	2(1)	3(1)
O(1')	22(1)	32(1)	20(1)	0(1)	-1(1)	-7(1)
O(1)	20(1)	45(1)	22(1)	-6(1)	-1(1)	7(1)
C(1)	20(1)	16(1)	21(1)	-1(1)	4(1)	-1(1)
C(2)	24(1)	24(1)	28(1)	2(1)	6(1)	4(1)
C(3)	24(1)	30(1)	37(1)	-1(1)	14(1)	5(1)
C(4)	30(1)	29(1)	28(1)	-2(1)	15(1)	-1(1)
C(5)	32(1)	32(1)	17(1)	0(1)	6(1)	-6(1)
C(6)	32(1)	32(1)	20(1)	6(1)	0(1)	-1(1)
C(7)	23(1)	26(1)	24(1)	3(1)	1(1)	1(1)
C(8)	19(1)	20(1)	18(1)	0(1)	3(1)	-4(1)
C(9)	20(1)	18(1)	20(1)	-2(1)	4(1)	-3(1)
C(10)	26(1)	22(1)	23(1)	-3(1)	7(1)	-3(1)
C(11)	20(1)	18(1)	21(1)	-1(1)	3(1)	3(1)
C(12)	17(1)	18(1)	19(1)	-1(1)	3(1)	2(1)
C(13)	24(1)	19(1)	21(1)	0(1)	2(1)	3(1)
C(14)	23(1)	23(1)	27(1)	2(1)	4(1)	-1(1)
C(15)	20(1)	24(1)	20(1)	1(1)	4(1)	3(1)
C(16)	31(1)	26(1)	24(1)	-6(1)	3(1)	9(1)
C(17)	26(1)	50(1)	25(1)	-4(1)	8(1)	7(1)
C(18)	27(1)	39(1)	28(1)	6(1)	10(1)	-4(1)
C(19)	36(1)	41(1)	24(1)	10(1)	9(1)	3(1)
C(20)	24(1)	35(1)	18(1)	2(1)	1(1)	5(1)
C(21)	30(1)	36(1)	21(1)	-7(1)	1(1)	4(1)
C(1')	18(1)	18(1)	20(1)	2(1)	3(1)	3(1)
C(2')	19(1)	20(1)	21(1)	1(1)	1(1)	1(1)
C(3')	19(1)	20(1)	26(1)	3(1)	4(1)	-1(1)
C(4')	24(1)	21(1)	22(1)	5(1)	4(1)	3(1)
C(5')	33(1)	32(1)	21(1)	0(1)	1(1)	1(1)
C(6')	32(1)	42(1)	25(1)	-7(1)	-4(1)	-4(1)
C(7')	23(1)	34(1)	37(1)	-9(1)	2(1)	-6(1)
C(8')	21(1)	25(1)	28(1)	-3(1)	4(1)	-1(1)
C(9')	17(1)	18(1)	23(1)	0(1)	1(1)	3(1)
C(10')	20(1)	21(1)	22(1)	1(1)	1(1)	4(1)

Table S29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **32f**.

	x	y	z	U(eq)
H(2)	4195	4969	4301	30
H(3)	3289	4560	5945	35
H(4)	4356	3444	7529	34
H(5)	6128	2107	8449	32
H(6)	7950	1001	8365	34
H(7)	8816	1073	6661	30
H(13A)	10403	-333	3709	26
H(13B)	9048	-804	3348	26
H(14A)	10056	3559	2927	29
H(14B)	11029	2388	3455	29
H(15A)	7511	1099	2523	26
H(15B)	7893	2769	2364	26
H(16)	10206	-1558	1897	33
H(17A)	11171	265	887	40
H(17B)	11689	345	2208	40
H(18)	11226	2787	1487	37
H(19A)	9187	3430	829	40
H(19B)	9605	2171	32	40
H(20)	7694	1541	553	31
H(21A)	8979	-494	280	35
H(21B)	8169	-907	1232	35
H(3')	8351	6504	2872	26
H(4')	7341	5950	1083	27
H(5')	5672	4662	-153	34
H(6')	4031	3095	-339	41
H(7')	3426	1999	1298	38
H(8')	4378	2564	3109	30
H(1)	7472(14)	2362(18)	4049(14)	25(4)
H(1')	8610(20)	6150(30)	4818(18)	63(6)

Table S30. Torsion angles [deg] for **32f**.

C(9)-C(1)-C(2)-C(3)	2.3(2)
C(1')-C(1)-C(2)-C(3)	-174.52(13)
C(1)-C(2)-C(3)-C(4)	2.5(2)
C(2)-C(3)-C(4)-C(10)	-3.8(2)
C(10)-C(5)-C(6)-C(7)	-1.2(2)
C(5)-C(6)-C(7)-C(8)	1.6(2)
C(6)-C(7)-C(8)-N(1)	-171.60(12)
C(6)-C(7)-C(8)-C(9)	1.27(19)
C(11)-N(1)-C(8)-C(7)	-22.29(19)
C(11)-N(1)-C(8)-C(9)	164.64(12)
C(7)-C(8)-C(9)-C(10)	-4.24(18)
N(1)-C(8)-C(9)-C(10)	168.71(11)
C(7)-C(8)-C(9)-C(1)	179.19(12)
N(1)-C(8)-C(9)-C(1)	-7.86(18)
C(2)-C(1)-C(9)-C(8)	170.87(12)
C(1')-C(1)-C(9)-C(8)	-12.6(2)
C(2)-C(1)-C(9)-C(10)	-5.66(18)
C(1')-C(1)-C(9)-C(10)	170.82(12)
C(3)-C(4)-C(10)-C(5)	-176.79(14)
C(3)-C(4)-C(10)-C(9)	0.2(2)
C(6)-C(5)-C(10)-C(4)	174.99(13)
C(6)-C(5)-C(10)-C(9)	-2.0(2)
C(8)-C(9)-C(10)-C(4)	-172.41(12)
C(1)-C(9)-C(10)-C(4)	4.47(18)
C(8)-C(9)-C(10)-C(5)	4.60(17)
C(1)-C(9)-C(10)-C(5)	-178.53(12)
C(8)-N(1)-C(11)-O(1)	-8.7(2)
C(8)-N(1)-C(11)-C(12)	169.56(12)
O(1)-C(11)-C(12)-C(15)	-179.61(12)
N(1)-C(11)-C(12)-C(15)	2.08(16)
O(1)-C(11)-C(12)-C(14)	-57.78(16)
N(1)-C(11)-C(12)-C(14)	123.91(12)
O(1)-C(11)-C(12)-C(13)	60.39(16)
N(1)-C(11)-C(12)-C(13)	-117.92(12)
C(11)-C(12)-C(13)-C(16)	-176.67(10)
C(15)-C(12)-C(13)-C(16)	59.33(13)
C(14)-C(12)-C(13)-C(16)	-58.75(13)
C(11)-C(12)-C(14)-C(18)	174.98(11)
C(15)-C(12)-C(14)-C(18)	-59.60(13)
C(13)-C(12)-C(14)-C(18)	58.27(13)
C(11)-C(12)-C(15)-C(20)	-178.85(11)
C(14)-C(12)-C(15)-C(20)	59.10(13)
C(13)-C(12)-C(15)-C(20)	-59.50(14)
C(12)-C(13)-C(16)-C(17)	60.24(14)
C(12)-C(13)-C(16)-C(21)	-60.36(15)
C(13)-C(16)-C(17)-C(18)	-61.45(14)
C(21)-C(16)-C(17)-C(18)	58.99(14)
C(16)-C(17)-C(18)-C(14)	61.23(14)
C(16)-C(17)-C(18)-C(19)	-58.81(14)
C(12)-C(14)-C(18)-C(17)	-59.63(14)
C(12)-C(14)-C(18)-C(19)	60.80(15)
C(17)-C(18)-C(19)-C(20)	59.54(15)
C(14)-C(18)-C(19)-C(20)	-60.54(16)
C(18)-C(19)-C(20)-C(21)	-60.38(15)
C(18)-C(19)-C(20)-C(15)	59.76(15)
C(12)-C(15)-C(20)-C(21)	60.50(14)
C(12)-C(15)-C(20)-C(19)	-59.68(14)
C(19)-C(20)-C(21)-C(16)	60.34(14)
C(15)-C(20)-C(21)-C(16)	-59.77(15)
C(17)-C(16)-C(21)-C(20)	-59.77(14)

C(13)-C(16)-C(21)-C(20)	60.15(15)
C(2)-C(1)-C(1')-C(2')	114.48(13)
C(9)-C(1)-C(1')-C(2')	-62.12(17)
C(2)-C(1)-C(1')-C(9')	-58.95(16)
C(9)-C(1)-C(1')-C(9')	124.45(13)
C(9')-C(1')-C(2')-O(1')	178.59(11)
C(1)-C(1')-C(2')-O(1')	5.03(17)
C(9')-C(1')-C(2')-C(3')	-1.19(18)
C(1)-C(1')-C(2')-C(3')	-174.76(12)
O(1')-C(2')-C(3')-C(4')	-177.38(12)
C(1')-C(2')-C(3')-C(4')	2.40(19)
C(2')-C(3')-C(4')-C(10')	-1.5(2)
C(10')-C(5')-C(6')-C(7')	-1.4(2)
C(5')-C(6')-C(7')-C(8')	2.1(2)
C(6')-C(7')-C(8')-C(9')	-0.1(2)
C(7')-C(8')-C(9')-C(10')	-2.3(2)
C(7')-C(8')-C(9')-C(1')	179.74(13)
C(2')-C(1')-C(9')-C(8')	177.00(12)
C(1)-C(1')-C(9')-C(8')	-9.53(19)
C(2')-C(1')-C(9')-C(10')	-0.88(18)
C(1)-C(1')-C(9')-C(10')	172.59(11)
C(6')-C(5')-C(10')-C(4')	178.03(13)
C(6')-C(5')-C(10')-C(9')	-1.1(2)
C(3')-C(4')-C(10')-C(5')	-179.70(13)
C(3')-C(4')-C(10')-C(9')	-0.60(19)
C(8')-C(9')-C(10')-C(5')	2.91(18)
C(1')-C(9')-C(10')-C(5')	-179.11(12)
C(8')-C(9')-C(10')-C(4')	-176.21(12)
C(1')-C(9')-C(10')-C(4')	1.77(18)

Symmetry transformations used to generate equivalent atoms:

Table S31. Hydrogen bonds for **32f** [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1')-H(1')...O(1)#1	0.98(2)	1.68(2)	2.6544(13)	173(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y+1/2,-z+1