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Supplemental information

Crystal structure determination of 4b (PD-089828).

The title compound crystallized from aqueous ethanol as colorless rods. The crystals are triclinic, space group P1_bar, with unit cell dimensions; a=11.102(9), b=12.010(2), c=16.289(3) Å, α = 78.24(2)°, β = 79.50(2)°, γ = 79.31(3)°, z =2;V = 2066.1(3)° Å^3. Lattice constants and intensity data were measured using graphite monochromated Cu Kα radiation, lambda = 1.54184 Å, on a Enraf-Nonius CAD-4 diffractometer. A total of 8835 reflections were measured, of which 8413 were unique and not systematically absent. The structure was determined using SIR-92 and refined by full matrix least squares using 6519 reflections with I/sigma(I)>3.0. Heavy atoms were refined using anisotropic temperature factors. Calculated positions and isotropic temperature factors for hydrogen atoms were included in structure factor calculations, but were not refined. The final difference map was 1.2 e/ Å^3.

Table of Positional Parameters and Their Estimated Standard Deviations:

Atom	x	y	z	B(A2)
CL1	0.8778(1)	0.37719(8)	0.68601(6)	8.26(2)
CL1'	0.08490(8)	0.59182(8)	0.58798(7)	7.02(2)
CL2	0.67956(8)	0.51810(7)	0.98194(5)	5.67(2)
CL2'	0.55564(6)	0.38636(7)	0.61869(5)	5.35(2)
O1	0.5037(2)	0.7829(2)	0.7448(2)	5.61(5)
O1'	0.3398(2)	0.3316(1)	0.8927(1)	4.53(4)
O2	0.4826(2)	0.5289(2)	0.8009(1)	5.29(5)
N1	1.2299(2)	0.6693(2)	0.8214(1)	4.10(5)

N1'	0.0946(2)	0.1163(2)	0.5120(1)	3.93(4)
N2	1.0564(2)	0.7976(2)	0.7672(1)	3.18(4)
N2'	0.1386(2)	0.0786(2)	0.6560(1)	3.53(4)
N3	0.8750(2)	0.7321(2)	0.7643(1)	3.19(4)
N3'	0.2285(2)	0.2055(2)	0.7048(1)	3.36(4)
N4	1.2384(2)	0.8604(2)	0.7686(2)	4.41(5)
N4'	0.0432(2)	-0.0427(2)	0.6072(1)	4.43(5)
N5	0.6874(2)	0.6733(2)	0.7646(1)	3.84(4)
N5'	0.3103(2)	0.3330(2)	0.7598(1)	3.68(4)
N6	0.6758(2)	0.8701(2)	0.7070(1)	3.84(4)
N6'	0.2472(2)	0.1882(2)	0.8706(1)	4.04(4)
C1	1.1641(2)	0.5853(2)	0.8382(2)	4.03(5)
C1'	0.1451(2)	0.2103(2)	0.4970(2)	3.80(5)
C2	1.1710(2)	0.7748(2)	0.7858(2)	3.40(5)
C2'	0.0934(2)	0.0533(2)	0.5929(2)	3.44(5)
C3	0.9912(2)	0.7090(2)	0.7842(1)	2.98(4)
C3'	0.1867(2)	0.1778(2)	0.6394(1)	3.15(4)
C4	0.8077(2)	0.6479(2)	0.7816(1)	3.12(4)
C4'	0.2724(2)	0.3040(2)	0.6923(1)	3.18(4)
C5	0.8529(2)	0.5316(2)	0.8176(2)	3.21(4)
C5'	0.2814(2)	0.3821(2)	0.6130(1)	3.26(5)
C6	0.9699(2)	0.5098(2)	0.8366(2)	3.74(5)
C6'	0.2411(2)	0.3514(2)	0.5475(1)	3.49(5)
C7	1.0427(2)	0.5981(2)	0.8212(2)	3.27(5)

C7'	0.1926(2)	0.2481(2)	0.5588(1)	3.35(5)
C8	0.7760(2)	0.4380(2)	0.8379(2)	3.49(5)
C8'	0.3220(2)	0.4955(2)	0.6039(1)	3.39(5)
C9	0.7850(3)	0.3584(2)	0.7846(2)	4.81(6)
C9'	0.2390(3)	0.5976(2)	0.5923(2)	4.39(6)
C10	0.7202(3)	0.2665(2)	0.8071(3)	6.46(8)
C10'	0.2725(4)	0.7045(2)	0.5844(2)	5.78(8)
C11	0.6473(3)	0.2514(2)	0.8836(3)	6.40(8)
C11'	0.3910(4)	0.7108(2)	0.5909(2)	6.22(8)
C12	0.6350(3)	0.3259(2)	0.9392(2)	5.39(7)
C12'	0.4776(3)	0.6148(2)	0.6025(2)	5.49(6)
C13	0.6988(2)	0.4190(2)	0.9149(2)	4.00(5)
C13'	0.4438(2)	0.5073(2)	0.6076(2)	3.93(5)
C14	0.6153(2)	0.7801(2)	0.7390(2)	3.82(5)
C14'	0.3002(2)	0.2832(2)	0.8462(2)	3.44(5)
C15	0.6149(2)	0.9894(2)	0.6822(2)	4.07(5)
C15'	0.2164(3)	0.1306(2)	0.9587(2)	4.80(6)
C16	0.5372(3)	0.9969(3)	0.6132(2)	6.45(8)
C16'	0.1680(4)	0.0232(3)	0.9531(3)	8.4(1)
C17	0.5374(3)	1.0342(3)	0.7577(2)	6.04(8)
C17'	0.3318(4)	0.0974(4)	1.0017(3)	8.9(1)
C18	0.7211(3)	1.0590(2)	0.6476(2)	5.65(8)
C18'	0.1202(5)	0.2064(4)	1.0068(3)	9.4(1)
H1	1.201	0.511	0.863	5.3*

H1'	0.150	0.255	0.441	5.0*
H6	1.003	0.434	0.861	4.9*
H6'	0.246	0.401	0.494	4.6*
H10	0.727	0.213	0.769	8.3*
H10'	0.214	0.773	0.575	7.5*
H11	0.604	0.187	0.899	8.4*
H11'	0.414	0.784	0.587	8.2*
H12	0.584	0.314	0.992	7.1*
H12'	0.560	0.621	0.607	7.1*
H21	0.470	0.481	0.835	6.9*
H22	0.423	0.578	0.808	06.9*
H4na	1.309	0.836	0.774	5.8*
H4na'	0.039	-0.077	0.654	5.8*
H4nb'	0.010	-0.061	0.569	5.8*
H4nb	1.196	0.935	0.743	5.8*
H5n'	0.341	0.392	0.756	4.8*
H5n	0.641	0.633	0.783	5.0*
H6n'	0.219	0.161	0.829	5.3*
H6n	0.766	0.862	0.717	5.0*
H16a'	0.105	0.043	0.918	10.5*
H16a	0.590	0.972	0.565	8.4*
H16b	0.499	1.074	0.598	8.4*
H16b'	0.234	-0.030	0.929	10.5*
H16c	0.476	0.948	0.632	8.4*

H16c'	0.135	-0.012	1.008	10.5*
H17a	0.500	1.112	0.742	7.9*
H17a'	0.352	0.163	1.016	11.6*
H17b	0.589	1.031	0.800	7.9*
H17b'	0.399	0.065	0.964	11.6*
H17c	0.474	0.988	0.782	7.9*
H17c'	0.316	0.041	1.051	11.6*
H18a	0.765	1.034	0.597	7.4*
H18a'	0.089	0.165	1.059	12.0*
H18b	0.776	1.046	0.688	7.4*
H18b'	0.156	0.269	1.016	12.0*
H18c	0.689	1.139	0.635	7.4*
H18c'	0.055	0.239	0.974	12.0*

*Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: (4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)].

Table of Bond Distances in Angstroms:

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
CL1	C9	1.740(3)	N5'	C4'	1.373(3)
CL1'	C9'	1.740(3)	N5'	C14'	1.406(3)
CL2	C13	1.733(3)	N6	C14	1.343(3)
CL2'	C13'	1.729(2)	N6	C15	1.475(3)
O1	C14	1.220(3)	N6'	C14'	1.336(3)
O1'	C14'	1.224(3)	N6'	C15'	1.470(3)
N1	C1	1.309(3)	C1	C7	1.400(3)
N1	C2	1.380(3)	C1'	C7'	1.403(4)
N1'	C1'	1.312(3)	C3	C7	1.407(3)

N1'	C2'	1.379(3)	C3'	C7'	1.407(3)
N2	C2	1.328(3)	C4	C5	1.436(3)
N2	C3	1.351(3)	C4'	C5'	1.432(3)
N2'	C2'	1.332(4)	C5	C6	1.356(3)
N2'	C3'	1.353(3)	C5	C8	1.484(3)
N3	C3	1.352(3)	C5'	C6'	1.366(4)
N3	C4	1.322(3)	C5'	C8'	1.484(3)
N3'	C3'	1.358(3)	C6	C7	1.407(3)
N3'	C4'	1.326(3)	C6'	C7'	1.408(4)
N4	C2	1.337(3)	C8	C9	1.397(4)
N4'	C2'	1.332(3)	C8	C13	1.387(3)
N5	C4	1.380(3)	C8'	C9'	1.392(3)
N5	C14	1.407(3)	C8'	C13'	1.399(4)
C9	C10	1.380(4)	C12'	C13'	1.393(4)
C9'	C10'	1.377(4)	C15	C16	1.515(5)
C10	C11	1.355(5)	C15	C17	1.502(4)
C10'	C11'	1.356(6)	C15	C18	1.529(4)
C11	C12	1.370(5)	C15'	C17'	1.511(5)
C11'	C12'	1.362(4)	C15'	C16'	1.522(6)
C12	C13	1.386(4)	C15'	C18'	1.486(5)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees:

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
C1	N1	C2	115.4(2)	N2'	C3'	C7'	121.7(2)
C1'	N1'	C2'	115.9(2)	N3'	C3'	C7'	122.1(2)
C2	N2	C3	117.1(2)	N3	C4	N5	118.3(2)
C2'	N2'	C3'	116.4(2)	N3	C4	C5	123.5(2)

C3	N3	C4	118.6(2)	N5	C4	C5	118.3(2)
C3'	N3'	C4'	118.3(2)	N3'	C4'	N5'	117.8(2)
C4	N5	C14	130.3(2)	N3'	C4'	C5'	123.9(2)
C4'	N5'	C14'	132.0(2)	N5'	C4'	C5'	118.4(2)
C14	N6	C15	124.5(2)	C4	C5	C6	117.1(2)
C14'	N6'	C15'	125.6(2)	C4	C5	C8	123.1(2)
N1	C1	C7	123.8(2)	C6	C5	C8	119.8(2)
N1'	C1'	C7'	123.2(2)	C4'	C5'	C6'	116.8(2)
N1	C2	N2	126.2(2)	C4'	C5'	C8'	121.8(2)
N1	C2	N4	115.3(2)	C6'	C5'	C8'	121.2(2)
N2	C2	N4	118.5(2)	C5	C6	C7	120.8(2)
N1'	C2'	N2'	126.4(2)	C5'	C6'	C7'	120.9(2)
N1'	C2'	N4'	115.4(2)	C1	C7	C3	116.4(2)
N2'	C2'	N4'	118.2(2)	C1	C7	C6	125.6(2)
N2	C3	N3	117.0(2)	C3	C7	C6	118.0(2)
N2	C3	C7	121.0(2)	C1'	C7'	C3'	116.4(2)
N3	C3	C7	121.9(2)	C1'	C7'	C6'	125.6(2)
N2'	C3'	N3'	116.3(2)	C3'	C7'	C6'	117.9(2)
C5	C8	C9	122.3(2)	CL2'	C13'	C8'	119.7(2
C5	C8	C13	121.3(2)	CL2'	C13'	C12'	118.9(2)
C9	C8	C13	116.2(2)	C8'	C13'	C12'	121.4(2)
C5'	C8'	C9'	121.3(2)	O1	C14	N5	117.7(2)
C5'	C8'	C13'	122.9(2)	O1	C14	N6	125.1(2)
C9'	C8'	C13'	115.8(2)	N5	C14	N6	117.2(2)
CL1	C9	C8	119.2(2)	O1'	C14'	N5'	117.0(2)
CL1	C9	C10	119.0(3)	O1'	C14'	N6'	125.7(2)
C8	C9	C10	121.8(3)	N5'	C14'	N6'	117.3(2)
CL1'	C9'	C8'	119.3(2)	N6	C15	C16	110.8(2)
CL1'	C9'	C10'	117.6(2)	N6	C15	C17	110.8(2)
C8'	C9'	C10'	123.2(3)	N6	C15	C18	105.1(2)
C9	C10	C11	119.4(3)	C16	C15	C17	110.8(2)
C9'	C10'	C11'	118.6(3)	C16	C15	C18	109.6(2)

C10	C11	C12	121.7(3)	C17	C15	C18	109.7(3)
C10'	C11'	C12'	121.8(3)	N6'	C15'	C16'	105.7(3)
C11	C12	C13	118.1(3)	N6'	C15'	C17'	110.4(3)
C11'	C12'	C13'	119.2(3)	N6'	C15'	C18'	110.5(2)
CL2	C13	C8	118.1(2)	C16'	C15'	C17'	109.7(3)
CL2	C13	C12	119.1(2)	C16'	C15'	C18'	110.6(3)
C8	C13	C12	122.7(3)	C17'	C15'	C18'	110.0(3)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Torsion Angles in Degrees

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C2	N1	C1	C7	0.79 (0.38)
C1	N1	C2	N2	-0.43 (0.38)
C1	N1	C2	N4	-179.89 (0.26)
C2'	N1'	C1'	C7'	-1.58 (0.36)
C1'	N1'	C2'	N2'	-0.35 (0.36)
C1'	N1'	C2'	N4'	-179.29 (0.23)
C3	N2	C2	N1	-0.33 (0.36)
C3	N2	C2	N4	179.12 (0.21)
C2	N2	C3	N3	-179.22 (0.20)
C2	N2	C3	C7	0.75 (0.32)
C3'	N2'	C2'	N1'	2.20 (0.35)
C3'	N2'	C2'	N4'	-178.88 (0.21)
C2'	N2'	C3'	N3'	177.61 (0.20)
C2'	N2'	C3'	C7'	-2.19 (0.33)
C4	N3	C3	N2	-178.73 (0.20)
C4	N3	C3	C7	1.31 (0.32)
C3	N3	C4	N5	177.13(0.20)
C3	N3	C4	C5	-2.54 (0.33)
C4'	N3'	C3'	N2'	-177.68 (0.20)

C4'	N3'	C3'	C7'	2.12 (0.33)
C3'	N3'	C4'	N5'	177.77 (0.20)
C3'	N3'	C4'	C5'	-1.52 (0.34)
C14	N5	C4	N3	-7.88 (0.38)
C14	N5	C4	C5	171.80 (0.24)
C4	N5	C14	O1	-165.04 (0.26)
C4	N5	C14	N6	17.47 (0.39)
C14'	N5'	C4'	N3'	-7.87 (0.38)
C14'	N5'	C4'	C5'	171.46 (0.23)
C4'	N5'	C14'	O1'	-177.46 (0.24)
C4'	N5'	C14'	N6'	1.81 (0.38)
C15	N6	C14	O1	6.76 (0.42)
C15	N6	C14	N5	-175.96 (0.22)
C14	N6	C15	C16	-60.21 (0.34)
C14	N6	C15	C17	63.19 (0.33)
C14	N6	C15	C18	-178.46 (0.25)
C15'	N6'	C14'	O1'	5.95 (0.42)
C15'	N6'	C14'	N5'	-173.25 (0.24)
C14'	N6'	C15'	C16'	-175.69 (0.27)
C14'	N6'	C15'	C17'	-57.22 (0.36)
C14'	N6'	C15'	C18'	64.69 (0.39)
N1	C1	C7	C3	-0.40 (0.38)
N1	C1	C7	C6	178.66 (0.25)
N1'	C1'	C7'	C3'	1.50 (0.37)
N1'	C1'	C7'	C6'	-176.13 (0.24)
N2	C3	C7	C1	-0.42 (0.33)
N2	C3	C7	C6	-179.55 (0.21)
N3	C3	C7	C1	179.54 (0.21)
N3	C3	C7	C6	0.41 (0.33)
N2'	C3'	C7'	C1'	0.50 (0.34)
N2'	C3'	C7'	C6'	178.32 (0.22)
N3'	C3'	C7'	C1'	-179.28 (0.22)

N3'	C3'	C7'	C6'	-1.46 (0.34)
N3	C4	C5	C6	1.98 (0.35)
N3	C4	C5	C8	179.17 (0.22)
N5	C4	C5	C6	-177.69 (0.22)
N5	C4	C5	C8	-0.50 (0.34)
N3'	C4'	C5'	C6'	0.28 (0.36)
N3'	C4'	C5'	C8'	175.09 (0.22)
N5'	C4'	C5'	C6'	-179.01 (0.22)
N5'	C4'	C5'	C8'	-4.20 (0.34)
C4	C5	C6	C7	-0.14 (0.36)
C8	C5	C6	C7	-177.43 (0.22)
C4	C5	C8	C9	99.73 (0.30)
C4	C5	C8	C13	-86.03 (0.31)
C6	C5	C8	C9	-83.16 (0.32)
C6	C5	C8	C13	91.08 (0.30)
C4'	C5'	C6'	C7'	0.41 (0.35)
C8'	C5'	C6'	C7'	-174.44 (0.22)
C4'	C5'	C8'	C9'	-109.05 (0.28)
C4'	C5'	C8'	C13'	69.88 (0.32)
C6'	C5'	C8'	C9'	65.53 (0.33)
C6'	C5'	C8'	C13'	-115.53 (0.27)
C5	C6	C7	C1	-180.00 (0.40)
C5	C6	C7	C3	-0.96 (0.36)
C5'	C6'	C7'	C1'	177.76 (0.24)
C5'	C6'	C7'	C3'	0.16 (0.35)
C5	C8	C9	CL1	-6.52 (0.35)
C5	C8	C9	C10	174.84 (0.27)
C13	C8	C9	CL1	178.96 (0.20)
C13	C8	C9	C10	0.33 (0.41)
C5	C8	C13	CL2	7.82 (0.32)
C5	C8	C13	C12	-173.65 (0.25)
C9	C8	C13	CL2	-177.60 (0.20)

C9	C8	C13	C12	0.93 (0.39)
C5'	C8'	C9'	CL1'	-0.29 (0.33)
C5'	C8'	C9'	C10'	179.38 (0.25)
C13'	C8'	C9'	CL1'	-179.30 (0.19)
C13'	C8'	C9'	C10'	0.37 (0.38)
C5'	C8'	C13'	CL2'	2.92 (0.32)
C5'	C8'	C13'	C12'	-177.23 (0.24)
C9'	C8'	C13'	CL2'	-178.08 (0.19)
C9'	C8'	C13'	C12'	1.77 (0.36)
CL1	C9	C10	C11	-179.78 (0.27)
C8	C9	C10	C11	-1.14 (0.49)
CL1'	C9'	C10'	C11'	177.49 (0.24)
C8'	C9'	C10'	C11'	-2.18 (0.45)
C9	C10	C11	C12	0.72 (0.52)
C9'	C10'	C11'	C12'	1.89 (0.48)
C10	C11	C12	C13	0.48 (0.50)
C10'	C11'	C12'	C13'	0.17 (0.47)
C11	C12	C13	CL2	177.17 (0.24)
C11	C12	C13	C8	-1.34 (0.44)
C11'	C12'	C13'	CL2'	177.78 (0.23)
C11'	C12'	C13'	C8'	-2.07 (0.41)