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J 3981-1

Figure Captions for Supporting Material

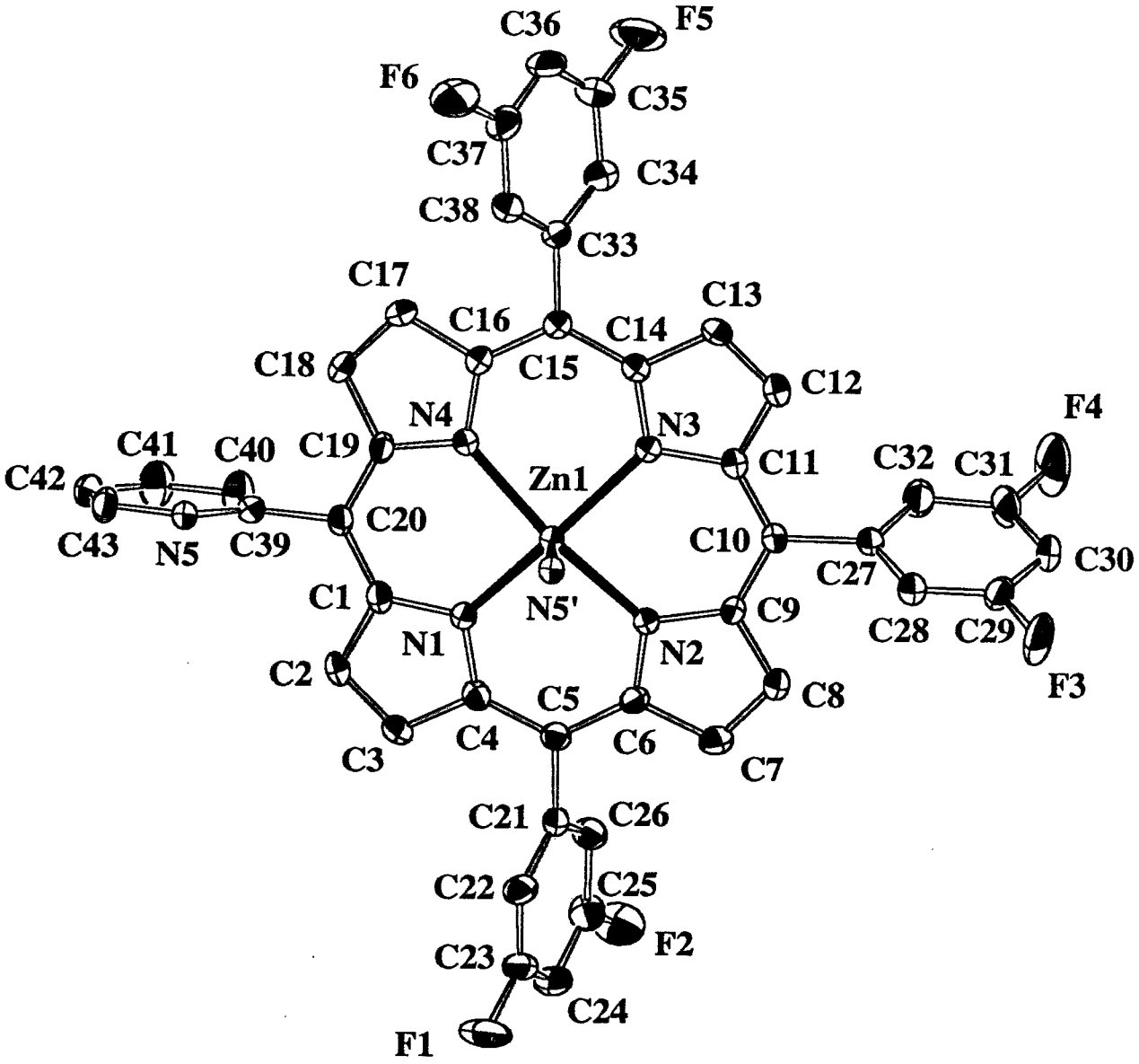
Figure S-1. Atom numbering scheme for the asymmetric unit of **3D**.

Figure S-2. Atom numbering scheme for the asymmetric unit of **1D.**

Figure S-3. Top view of **1D**.

Figure S-4. Side view of **1D**.

J3981-2



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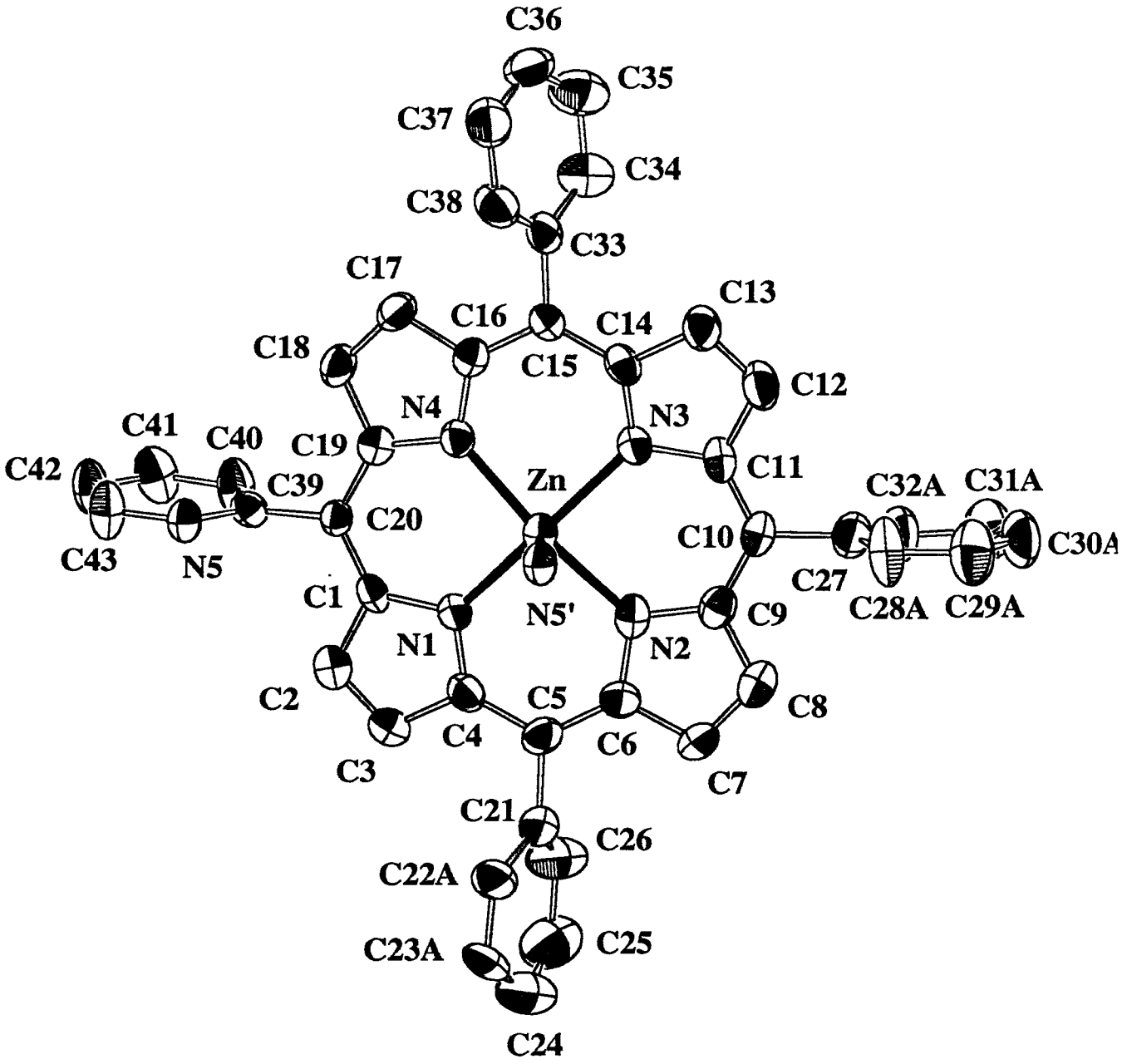
J3981-3



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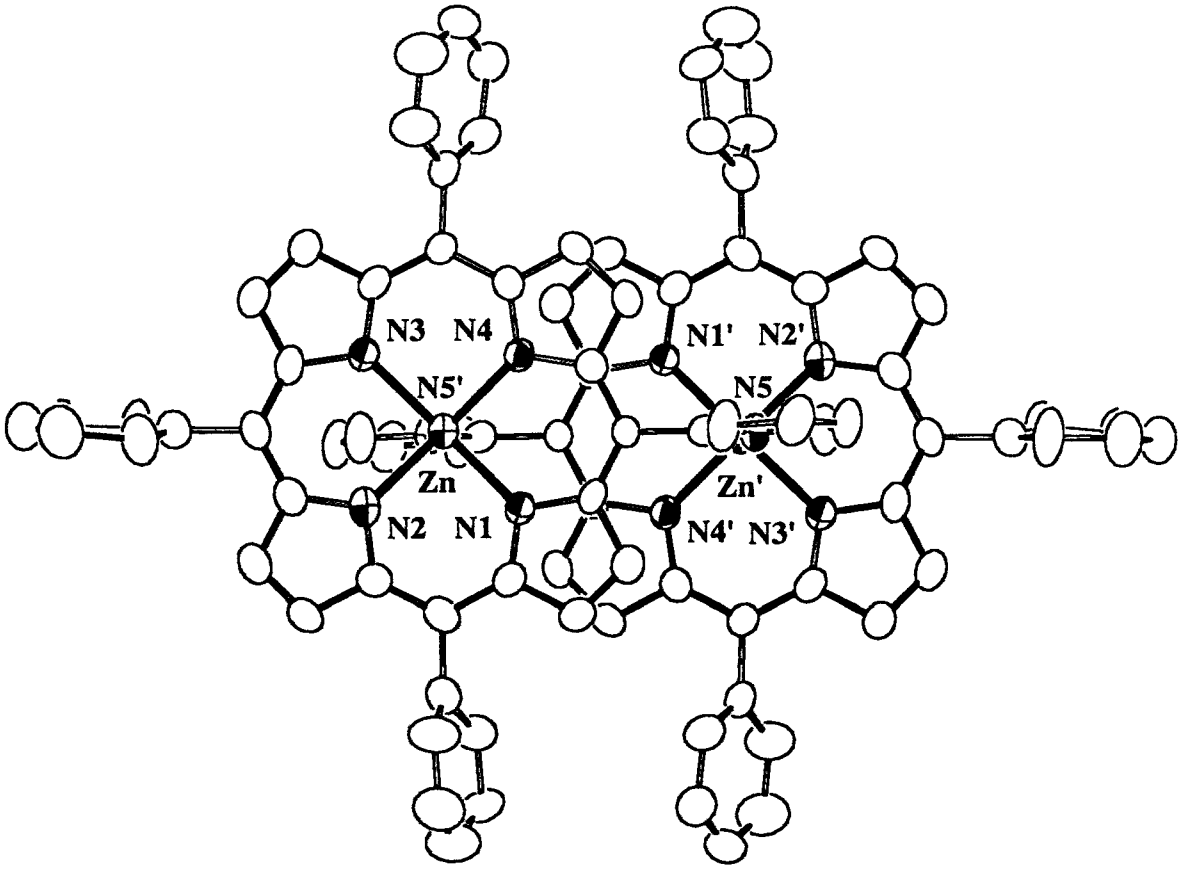
J3981-4



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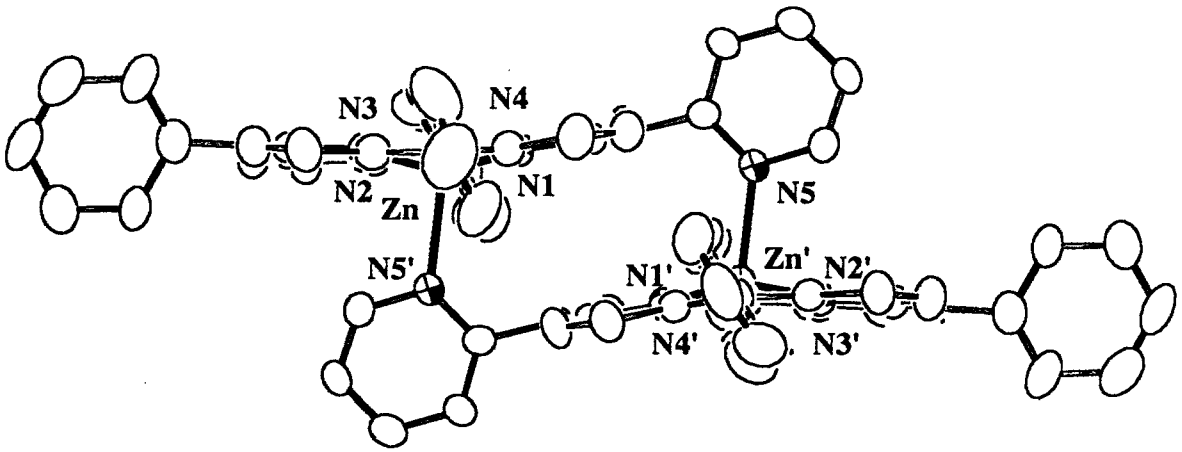

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J3981-6

Structure Solution and Refinement Details for **1D** and **3D**:

The crystal structures of **1D** and **3D** were solved by use of direct methods and Patterson methods, respectively. The structures of **1D** and **3D** were completed with difference-Fourier techniques, and refined using full-matrix least-squares on all F^2_{obs} data. Anisotropic displacement parameters were varied for all non-H atoms. The H atoms were placed on the external bisector of the C-C_H-C angle at a fixed distance of 0.95 Å, and their coordinates were allowed to "ride" on the coordinates of their bonded C atom, C_H. The H atom U_{ISO} values were set to equal 1.2 times that of C_H. The first two solvent molecules, C44A through Cl3A and C44B through Cl3B, were not related by the (1/2,1/2,0) inversion center, but were in sites of approximately half occupancy. These occupancies, with a sum constrained to 1.0, were refined to 0.441(3) for the molecule A and 0.559(3) for molecule B. The occupancy of the third solvent molecule, C45 through Cl6, was refined to 0.427(3). The presence of positional disorder in only two phenyl rings for **1D** and in the three (half-occupancy) solvent molecules for **3D** required the use of the following additional restraints:

Restraints for **1D**:

1. split positions were given for two C atoms (C22A, C22B, C23A, C23B) and respective H atoms of the C21-C26 phenyl ring and for four C atoms (C28A, C28B, C29A, C29B, C30A, C30B, C31A, C31B) and respective H atoms of the C27-C32 phenyl ring;
2. The C-C bond distances for all C atoms in the above two rings were restrained to a target value 1.39 Å with an estimated standard deviation 0.03 Å;
3. All phenyl and pyridyl C and N atoms were restrained with effective standard deviation 0.03 so that their Uij components approximated isotropic behavior (the corresponding isotropic U was free to vary);
4. For the set of disordered atoms (C22A through C22B and C28A through C31B), atoms closer than 1.7 Å were restrained with effective standard deviation 0.03 to have the same Uij components;
5. the following bonds (C - C) and distances (C...C) were restrained to be the same length:
   C22A - C23A and C22B - C23B
   C28A - C29A and C28B - C29B
   C29A - C30A and C29B - C30B
   C30A - C31A and C30B - C31B
   C28A...C30A and C28B...C30B
   C29A...C31A and C29B...C31B

Restraints for **3D**:

1. significantly separate positions were given for the two halves of one $CHCl_3$ solvent molecule (C45A through Cl3A *versus* C45B through Cl3B);
2. The C-Cl and Cl...Cl distances for each of these two half molecules were restrained to a target value 1.74 Å and 2.84 Å, respectively -- all with an estimated standard deviation 0.03 Å;
3. All solvent molecule atoms were restrained with effective standard deviation 0.03 so that their Uij components approximated isotropic behavior (the corresponding isotropic U was free to vary);
4. For the solvent molecules, all atoms closer than 1.7 Å were restrained with effective standard deviation 0.03 to have the same Uij components

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

Empirical formula	$C_{43}\ H_{27}\ N_5\ Zn$
Formula weight	679.07
Temperature	293(2) K
Radiation (type, wavelength)	Mo K_α, 0.71073 Å
Diffractometer, monochromator	CAD4, graphite
Standard reflections, no. & interval	3, 10800 s
Decay of standards	< 1 %
Crystal system, space group	monoclinic, $P2_1/c$
No. refl, θ range for cell det'n	25, 11.3 to 14.9 °
Unit cell dimensions a = 16.272(2) Å α = 90.00(2) ° b = 12.930(4) Å β = 115.22(1) ° c = 17.478(4) Å γ = 90.00(2) °	
Volume	3327(1) Å^3
Z	4
Density (calculated)	1.356 Mg/m^3
Density (measured)	1.36(1) Mg/m^3
Absorption coefficient	0.778 mm^{-1}
F(000)	1400
Crystal color, description	dark red, hexagonal plates
Crystal size	0.35 x 0.25 x 0.02 mm
θ range for data collection	2 to 20 °
Scan type, speeds	ω - 2θ, 1.0 to 5.5 ° min^{-1}
Scan ranges, apertures	0.65 + 0.35*tan*θ, 1.5 + 1.5*tan*θ
Index ranges	0<=h<=15, 0<=k<=12, -16<=l<=15

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Table S1. concluded for **1D**.

Reflections collected	3438
Absorption correction	Numerical grid
Max. and min. transmission	0.791 and 0.887
Independent reflections	3096 [R(int) = 0.031]
Observed reflections	2291
Refinement method (SHELXL93)	Full-matrix least-squares on F^2
Data / restraints / parameters	3096 / 312 / 489
Goodness-of-fit on F^2	1.044
Final R(F), wR(F^2) indices [I>2σ(I)]	0.041, 0.092
Final R(F), wR(F^2) indices (all I)	0.073, 0.099
Largest diff. peak and hole	0.3 and -0.3 e·Å^{-3}

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

	x	y	z	U(eq)
Zn	1083.7(3)	6533.0(4)	4599.3(3)	38.6(2)
N(1)	1375(3)	4970(3)	4782(2)	36(1)
N(2)	2461(3)	6769(3)	4937(2)	43(1)
N(3)	854(3)	7986(3)	4017(2)	38(1)
N(4)	-235(2)	6171(3)	3800(2)	38(1)
N(5)	-1105(2)	2912(3)	4195(2)	41(1)
C(1)	746(3)	4179(4)	4513(3)	36(1)
C(2)	1216(4)	3219(4)	4834(3)	51(2)
C(3)	2093(4)	3437(4)	5265(3)	55(2)
C(4)	2198(4)	4534(4)	5235(3)	42(1)
C(5)	3039(3)	5056(4)	5569(3)	45(1)
C(6)	3158(3)	6102(4)	5418(3)	44(1)
C(7)	4016(3)	6613(5)	5697(3)	52(1)
C(8)	3835(3)	7579(5)	5388(3)	54(2)
C(9)	2883(3)	7691(4)	4924(3)	42(1)
C(10)	2429(3)	8603(4)	4536(3)	44(1)
C(11)	1497(4)	8747(4)	4138(3)	42(1)
C(12)	1032(4)	9698(4)	3783(3)	56(2)
C(13)	141(4)	9513(4)	3466(3)	53(2)
C(14)	22(3)	8438(4)	3591(3)	39(1)
C(15)	-813(3)	7921(4)	3271(3)	37(1)
C(16)	-914(3)	6846(4)	3334(3)	39(1)
C(17)	-1743(3)	6282(4)	2885(3)	48(1)
C(18)	-1570(3)	5280(4)	3085(3)	48(1)
C(19)	-621(3)	5201(4)	3663(3)	36(1)
C(20)	-168(3)	4282(4)	4010(3)	32(1)
C(21)	3866(4)	4423(4)	6092(4)	56(2)
C(22A)	3976(9)	3964(13)	6842(8)	60(4)
C(23A)	4692(9)	3328(13)	7302(9)	74(5)
C(22B)	4217(13)	4590(22)	6981(11)	89(6)
C(23B)	4986(14)	3986(19)	7470(12)	93(6)
C(24)	5336(5)	3192(6)	7043(6)	106(3)
C(25)	5147(4)	3390(5)	6240(5)	93(2)
C(26)	4402(4)	4008(5)	5761(4)	78(2)
C(27)	3003(3)	9524(4)	4569(4)	55(2)
C(28A)	3210(10)	10208(10)	5284(10)	79(4)
C(29A)	3721(8)	11097(8)	5360(11)	84(4)
C(30A)	4024(8)	11273(10)	4748(10)	77(4)
C(31A)	3888(14)	10574(13)	4111(12)	88(5)
C(28B)	2938(16)	10466(16)	4823(20)	72(7)
C(29B)	3409(16)	11312(15)	4743(20)	73(6)
C(30B)	3887(20)	11224(21)	4265(22)	78(7)
C(31B)	4003(25)	10292(22)	3934(24)	80(8)

J398/-10

Table S2. concluded for **1D**.

C(32)	3414(4)	9607(5)	4050(4)	77(2)
C(33)	-1667(3)	8509(4)	2799(3)	42(1)
C(34)	-1840(4)	8975(5)	2035(4)	64(2)
C(35)	-2656(5)	9469(5)	1585(4)	79(2)
C(36)	-3308(4)	9475(5)	1874(5)	75(2)
C(37)	-3149(4)	9030(5)	2631(5)	71(2)
C(38)	-2323(4)	8558(4)	3098(4)	60(2)
C(39)	-715(3)	3314(4)	3723(3)	36(1)
C(40)	-835(4)	2872(4)	2974(3)	58(2)
C(41)	-1379(4)	2013(4)	2664(3)	62(2)
C(42)	-1767(4)	1588(4)	3142(3)	55(2)
C(43)	-1606(4)	2053(4)	3896(3)	59(2)

J398411

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

Zn-N(4)	2.053(4)	Zn-N(1)	2.070(4)
Zn-N(2)	2.082(4)	Zn-N(3)	2.094(4)
Zn-N(5)'	2.212(4)	N(1)-C(4)	1.355(6)
N(1)-C(1)	1.379(6)	N(2)-C(9)	1.381(6)
N(2)-C(6)	1.387(6)	N(3)-C(14)	1.366(6)
N(3)-C(11)	1.386(6)	N(4)-C(16)	1.371(6)
N(4)-C(19)	1.378(6)	N(5)-C(39)	1.342(5)
N(5)-C(43)	1.345(6)	N(5)-Zn'	2.212(4)
C(1)-C(20)	1.374(6)	C(1)-C(2)	1.441(7)
C(2)-C(3)	1.329(6)	C(3)-C(4)	1.432(7)
C(4)-C(5)	1.410(6)	C(5)-C(6)	1.407(7)
C(5)-C(21)	1.505(7)	C(6)-C(7)	1.430(7)
C(7)-C(8)	1.343(7)	C(8)-C(9)	1.417(6)
C(9)-C(10)	1.403(7)	C(10)-C(11)	1.385(6)
C(10)-C(27)	1.499(7)	C(11)-C(12)	1.439(7)
C(12)-C(13)	1.334(6)	C(13)-C(14)	1.434(7)
C(14)-C(15)	1.400(6)	C(15)-C(16)	1.409(6)
C(15)-C(33)	1.487(6)	C(16)-C(17)	1.438(6)
C(17)-C(18)	1.340(6)	C(18)-C(19)	1.443(6)
C(19)-C(20)	1.394(6)	C(20)-C(39)	1.494(6)
C(21)-C(26)	1.347(7)	C(21)-C(22B)	1.43(2)
C(21)-C(22A)	1.380(13)	C(22A)-C(23A)	1.372(12)
C(23A)-C(24)	1.318(14)	C(22B)-C(23B)	1.41(2)
C(23B)-C(24)	1.52(2)	C(24)-C(25)	1.328(9)
C(25)-C(26)	1.394(8)	C(27)-C(28B)	1.32(2)
C(27)-C(32)	1.341(7)	C(27)-C(28A)	1.448(12)
C(28A)-C(29A)	1.392(11)	C(29A)-C(30A)	1.375(13)
C(30A)-C(31A)	1.376(14)	C(31A)-C(32)	1.45(2)
C(28B)-C(29B)	1.38(2)	C(29B)-C(30B)	1.37(2)
C(30B)-C(31B)	1.38(2)	C(31B)-C(32)	1.38(2)
C(33)-C(38)	1.376(6)	C(33)-C(34)	1.381(7)
C(34)-C(35)	1.378(8)	C(35)-C(36)	1.354(8)
C(36)-C(37)	1.362(8)	C(37)-C(38)	1.381(7)
C(39)-C(40)	1.365(6)	C(40)-C(41)	1.380(7)
C(41)-C(42)	1.359(7)	C(42)-C(43)	1.368(7)

N(4)-Zn-N(1)	89.2(2)	N(4)-Zn-N(2)	155.8(1)
N(1)-Zn-N(2)	87.2(2)	N(4)-Zn-N(3)	87.5(2)
N(1)-Zn-N(3)	159.0(1)	N(2)-Zn-N(3)	87.4(2)
N(4)-Zn-N(5)'	108.0(1)	N(1)-Zn-N(5)'	105.1(2)
N(2)-Zn-N(5)'	96.0(1)	N(3)-Zn-N(5)'	95.6(1)
C(4)-N(1)-C(1)	107.2(4)	C(4)-N(1)-Zn	126.9(3)
C(1)-N(1)-Zn	125.7(3)	C(9)-N(2)-C(6)	105.3(4)
C(9)-N(2)-Zn	127.2(3)	C(6)-N(2)-Zn	125.7(3)
C(14)-N(3)-C(11)	106.7(4)	C(14)-N(3)-Zn	125.4(3)
C(11)-N(3)-Zn	126.6(3)	C(16)-N(4)-C(19)	106.5(4)
C(16)-N(4)-Zn	127.0(3)	C(19)-N(4)-Zn	126.4(3)
C(39)-N(5)-C(43)	116.7(4)	C(39)-N(5)-Zn'	129.8(3)
C(43)-N(5)-Zn'	113.5(3)	C(20)-C(1)-N(1)	126.1(4)

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Table S3. concluded for **1D**.

C(20)-C(1)-C(2)	125.6(5)	N(1)-C(1)-C(2)	108.3(4)
C(3)-C(2)-C(1)	107.5(5)	C(2)-C(3)-C(4)	107.8(5)
N(1)-C(4)-C(5)	125.8(5)	N(1)-C(4)-C(3)	109.2(4)
C(5)-C(4)-C(3)	124.8(5)	C(6)-C(5)-C(4)	124.7(5)
C(6)-C(5)-C(21)	118.6(4)	C(4)-C(5)-C(21)	116.6(5)
N(2)-C(6)-C(5)	124.7(5)	N(2)-C(6)-C(7)	110.3(5)
C(5)-C(6)-C(7)	124.9(5)	C(8)-C(7)-C(6)	106.1(5)
C(7)-C(8)-C(9)	108.9(5)	N(2)-C(9)-C(10)	124.9(4)
N(2)-C(9)-C(8)	109.4(5)	C(10)-C(9)-C(8)	125.7(5)
C(11)-C(10)-C(9)	126.4(4)	C(11)-C(10)-C(27)	116.3(5)
C(9)-C(10)-C(27)	117.3(4)	N(3)-C(11)-C(10)	125.1(5)
N(3)-C(11)-C(12)	108.5(4)	C(10)-C(11)-C(12)	126.4(5)
C(13)-C(12)-C(11)	107.7(5)	C(12)-C(13)-C(14)	107.7(5)
N(3)-C(14)-C(15)	125.5(5)	N(3)-C(14)-C(13)	109.3(4)
C(15)-C(14)-C(13)	125.0(5)	C(14)-C(15)-C(16)	124.4(4)
C(14)-C(15)-C(33)	119.7(4)	C(16)-C(15)-C(33)	115.9(4)
N(4)-C(16)-C(15)	125.7(4)	N(4)-C(16)-C(17)	109.4(4)
C(15)-C(16)-C(17)	124.9(5)	C(18)-C(17)-C(16)	107.7(4)
C(17)-C(18)-C(19)	107.1(4)	N(4)-C(19)-C(20)	125.7(4)
N(4)-C(19)-C(18)	109.3(4)	C(20)-C(19)-C(18)	125.1(5)
C(1)-C(20)-C(19)	126.1(4)	C(1)-C(20)-C(39)	117.5(4)
C(19)-C(20)-C(39)	116.1(4)	C(26)-C(21)-C(22B)	119.7(9)
C(26)-C(21)-C(22A)	113.0(8)	C(26)-C(21)-C(5)	122.1(5)
C(22B)-C(21)-C(5)	114.8(10)	C(22A)-C(21)-C(5)	122.1(7)
C(23A)-C(22A)-C(21)	123.3(12)	C(24)-C(23A)-C(22A)	118.6(11)
C(21)-C(22B)-C(23B)	115(2)	C(22B)-C(23B)-C(24)	120(2)
C(25)-C(24)-C(23A)	118.5(9)	C(25)-C(24)-C(23B)	115.0(9)
C(24)-C(25)-C(26)	119.8(7)	C(21)-C(26)-C(25)	121.8(6)
C(28B)-C(27)-C(32)	106.8(12)	C(32)-C(27)-C(28A)	122.3(7)
C(28B)-C(27)-C(10)	127.6(10)	C(32)-C(27)-C(10)	121.3(6)
C(28A)-C(27)-C(10)	115.5(7)	C(29A)-C(28A)-C(27)	119.8(10)
C(30A)-C(29A)-C(28A)	117.4(10)	C(31A)-C(30A)-C(29A)	122.2(11)
C(30A)-C(31A)-C(32)	121.6(13)	C(27)-C(28B)-C(29B)	125(2)
C(30B)-C(29B)-C(28B)	119(2)	C(29B)-C(30B)-C(31B)	123(2)
C(30B)-C(31B)-C(32)	106(2)	C(27)-C(32)-C(31B)	136.6(13)
C(27)-C(32)-C(31A)	115.0(9)	C(38)-C(33)-C(34)	118.4(5)
C(38)-C(33)-C(15)	120.4(5)	C(34)-C(33)-C(15)	121.1(5)
C(35)-C(34)-C(33)	120.2(5)	C(36)-C(35)-C(34)	120.5(6)
C(35)-C(36)-C(37)	120.3(6)	C(36)-C(37)-C(38)	119.7(6)
C(33)-C(38)-C(37)	120.8(5)	N(5)-C(39)-C(40)	121.0(4)
N(5)-C(39)-C(20)	119.3(4)	C(40)-C(39)-C(20)	119.6(4)
C(39)-C(40)-C(41)	121.3(5)	C(42)-C(41)-C(40)	118.2(5)
C(41)-C(42)-C(43)	117.8(5)	N(5)-C(43)-C(42)	124.9(5)

Symmetry transformations used to generate equivalent atoms:
' -x,-y+1,-z+1

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Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1D**. 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
Zn	40.7(4)	36.1(4)	40.7(4)	-2.3(3)	19.0(3)	-6.6(3)
N(1)	38(3)	32(3)	38(3)	1(2)	15(2)	-3(2)
N(2)	47(3)	42(3)	43(3)	-4(2)	23(2)	-11(3)
N(3)	41(3)	32(3)	43(3)	0(2)	21(2)	-2(3)
N(4)	40(3)	31(3)	43(3)	-2(2)	19(2)	-3(2)
N(5)	47(2)	35(3)	42(3)	-7(2)	22(2)	-10(2)
C(1)	49(4)	25(3)	36(3)	1(3)	19(3)	-5(3)
C(2)	52(4)	43(4)	57(4)	3(3)	24(3)	-6(3)
C(3)	48(4)	44(4)	68(4)	14(3)	18(3)	5(3)
C(4)	49(4)	37(4)	39(3)	7(3)	17(3)	-1(3)
C(5)	38(3)	58(4)	32(3)	2(3)	7(3)	-7(3)
C(6)	43(4)	48(4)	36(3)	5(3)	11(3)	-1(3)
C(7)	34(3)	53(4)	55(3)	0(3)	5(3)	-5(3)
C(8)	43(4)	56(4)	61(4)	-9(3)	21(3)	-13(3)
C(9)	41(4)	50(4)	41(3)	-5(3)	23(3)	-8(3)
C(10)	40(4)	46(4)	51(3)	-7(3)	25(3)	-12(3)
C(11)	51(4)	34(4)	53(3)	-4(3)	33(3)	-9(3)
C(12)	59(4)	35(4)	85(4)	3(3)	40(3)	-4(3)
C(13)	49(4)	33(4)	82(4)	-1(3)	32(3)	1(3)
C(14)	50(4)	28(4)	47(3)	0(3)	28(3)	3(3)
C(15)	42(3)	31(3)	38(3)	2(3)	17(3)	1(3)
C(16)	38(3)	42(4)	38(3)	-2(3)	18(3)	-5(3)
C(17)	32(3)	44(4)	58(3)	-4(3)	11(3)	-2(3)
C(18)	41(4)	37(4)	59(4)	-11(3)	14(3)	-10(3)
C(19)	40(3)	38(4)	33(3)	-7(3)	19(3)	-3(3)
C(20)	34(3)	31(4)	32(3)	-2(3)	13(3)	-5(3)
C(21)	44(4)	59(4)	57(4)	14(3)	14(3)	-7(3)
C(22A)	50(7)	74(9)	54(7)	26(7)	21(6)	4(7)
C(23A)	62(9)	69(11)	80(8)	51(8)	21(7)	13(7)
C(22B)	60(10)	137(16)	70(11)	45(12)	27(8)	16(12)
C(23B)	89(11)	122(14)	70(9)	55(10)	35(8)	-2(11)
C(24)	71(5)	113(7)	113(7)	53(6)	18(5)	20(5)
C(25)	70(5)	73(5)	115(6)	-27(5)	18(5)	11(4)
C(26)	65(4)	75(5)	68(4)	-5(4)	5(4)	18(4)
C(27)	46(4)	46(4)	76(4)	-3(3)	28(3)	-5(3)
C(28A)	108(9)	54(7)	103(10)	-17(7)	72(8)	-37(7)
C(29A)	99(8)	56(7)	113(10)	-21(7)	61(7)	-22(6)
C(30A)	70(7)	66(7)	115(9)	16(7)	61(8)	-11(6)
C(31A)	86(9)	100(12)	98(10)	11(10)	58(7)	-15(10)
C(28B)	70(11)	59(13)	114(14)	1(12)	64(11)	-13(10)
C(29B)	83(11)	49(10)	110(12)	3(11)	64(11)	-13(10)
C(30B)	82(11)	72(12)	91(14)	21(13)	49(11)	10(11)
C(31B)	54(12)	95(16)	100(16)	32(13)	41(10)	8(12)

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Table S4. concluded for **1D**.

C(32)	77(4)	85(5)	74(4)	12(4)	37(4)	-29(4)
C(33)	51(3)	30(3)	39(3)	-5(3)	14(3)	-7(3)
C(34)	66(4)	70(4)	51(4)	-3(3)	22(3)	15(4)
C(35)	83(5)	86(5)	51(4)	5(4)	13(4)	12(4)
C(36)	45(4)	53(4)	91(5)	-3(4)	-4(4)	4(3)
C(37)	58(4)	52(4)	114(6)	9(4)	46(4)	8(3)
C(38)	57(4)	56(4)	77(4)	22(3)	39(3)	13(3)
C(39)	42(3)	36(3)	30(3)	2(3)	15(3)	1(3)
C(40)	92(4)	46(4)	51(4)	-17(3)	43(3)	-26(3)
C(41)	98(4)	48(4)	49(4)	-13(3)	40(4)	-17(4)
C(42)	80(4)	41(3)	49(4)	-15(3)	32(3)	-27(3)
C(43)	80(4)	54(4)	57(4)	-13(3)	42(3)	-31(4)

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

	x	y	z	U(eq)
H(2)	953(4)	2566(4)	4754(3)	61
H(3)	2555(4)	2963(4)	5537(3)	66
H(7)	4585(3)	6334(5)	6027(3)	63
H(8)	4265(3)	8091(5)	5465(3)	64
H(12)	1303(4)	10328(4)	3775(3)	68
H(13)	-320(4)	9994(4)	3209(3)	64
H(17)	-2300(3)	6561(4)	2521(3)	58
H(18)	-1983(3)	4738(4)	2889(3)	58
H(22A)	3543(9)	4093(13)	7046(8)	72
H(23A)	4722(9)	2999(13)	7787(9)	88
H(22B)	3961(13)	5058(22)	7220(11)	106
H(23B)	5278(14)	4076(19)	8053(12)	112
H(24)	5910(5)	2962(6)	7415(6)	127
H(25)	5510(4)	3118(5)	5998(5)	112
H(26)	4273(4)	4137(5)	5197(4)	93
H(28A)	3002(10)	10053(10)	5690(10)	95
H(29A)	3852(8)	11554(8)	5807(11)	101
H(30A)	4332(8)	11884(10)	4765(10)	92
H(31A)	4105(14)	10726(13)	3710(12)	106
H(28B)	2544(16)	10568(16)	5076(20)	87
H(29B)	3402(16)	11933(15)	5009(20)	88
H(30B)	4145(20)	11815(21)	4158(22)	93
H(31B)	4395(25)	10155(22)	3685(24)	96
H(32)	3396(4)	9083(5)	3679(4)	93
H(34)	-1405(4)	8955(5)	1822(4)	76
H(35)	-2761(5)	9800(5)	1080(4)	95
H(36)	-3866(4)	9786(5)	1555(5)	90
H(37)	-3595(4)	9043(5)	2831(5)	86
H(38)	-2210(4)	8271(4)	3622(4)	72
H(40)	-545(4)	3156(4)	2665(3)	70
H(41)	-1478(4)	1732(4)	2142(3)	75
H(42)	-2130(4)	1001(4)	2963(3)	66
H(43)	-1862(4)	1752(4)	4227(3)	71

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Table S6. Torsion angles [°] for **1D**.

N(4)-Zn-N(1)-C(4)	175.7(4)	N(2)-Zn-N(1)-C(4)	19.6(4)
N(3)-Zn-N(1)-C(4)	94.8(5)	N(5)' -Zn-N(1)-C(4)	-75.9(4)
N(4)-Zn-N(1)-C(1)	-9.5(4)	N(2)-Zn-N(1)-C(1)	-165.6(4)
N(3)-Zn-N(1)-C(1)	-90.4(5)	N(5)' -Zn-N(1)-C(1)	98.9(4)
N(4)-Zn-N(2)-C(9)	93.0(5)	N(1)-Zn-N(2)-C(9)	174.8(4)
N(3)-Zn-N(2)-C(9)	15.2(4)	N(5)' -Zn-N(2)-C(9)	-80.3(4)
N(4)-Zn-N(2)-C(6)	-104.8(5)	N(1)-Zn-N(2)-C(6)	-22.9(4)
N(3)-Zn-N(2)-C(6)	177.4(4)	N(5)' -Zn-N(2)-C(6)	82.0(4)
N(4)-Zn-N(3)-C(14)	22.6(4)	N(1)-Zn-N(3)-C(14)	103.7(5)
N(2)-Zn-N(3)-C(14)	179.0(4)	N(5)' -Zn-N(3)-C(14)	-85.3(4)
N(4)-Zn-N(3)-C(11)	-172.2(4)	N(1)-Zn-N(3)-C(11)	-91.0(5)
N(2)-Zn-N(3)-C(11)	-15.8(4)	N(5)' -Zn-N(3)-C(11)	80.0(4)
N(1)-Zn-N(4)-C(16)	-175.4(4)	N(2)-Zn-N(4)-C(16)	-93.9(5)
N(3)-Zn-N(4)-C(16)	-16.2(4)	N(5)' -Zn-N(4)-C(16)	79.0(4)
N(1)-Zn-N(4)-C(19)	8.2(4)	N(2)-Zn-N(4)-C(19)	89.7(5)
N(3)-Zn-N(4)-C(19)	167.4(4)	N(5)' -Zn-N(4)-C(19)	-97.4(4)
C(4)-N(1)-C(1)-C(20)	-177.7(4)	Zn-N(1)-C(1)-C(20)	6.7(6)
C(4)-N(1)-C(1)-C(2)	1.0(5)	Zn-N(1)-C(1)-C(2)	-174.6(3)
C(20)-C(1)-C(2)-C(3)	177.7(4)	N(1)-C(1)-C(2)-C(3)	-1.0(5)
C(1)-C(2)-C(3)-C(4)	0.6(6)	C(1)-N(1)-C(4)-C(5)	174.6(4)
Zn-N(1)-C(4)-C(5)	-9.8(7)	C(1)-N(1)-C(4)-C(3)	-0.7(5)
Zn-N(1)-C(4)-C(3)	174.9(3)	C(2)-C(3)-C(4)-N(1)	0.0(6)
C(2)-C(3)-C(4)-C(5)	-175.3(5)	N(1)-C(4)-C(5)-C(6)	-5.9(8)
C(3)-C(4)-C(5)-C(6)	168.7(5)	N(1)-C(4)-C(5)-C(21)	176.9(5)
C(3)-C(4)-C(5)-C(21)	-8.5(7)	C(9)-N(2)-C(6)-C(5)	-177.3(5)
Zn-N(2)-C(6)-C(5)	17.3(7)	C(9)-N(2)-C(6)-C(7)	-0.5(5)
Zn-N(2)-C(6)-C(7)	-165.9(3)	C(4)-C(5)-C(6)-N(2)	1.7(8)
C(21)-C(5)-C(6)-N(2)	178.9(4)	C(4)-C(5)-C(6)-C(7)	-174.6(5)
C(21)-C(5)-C(6)-C(7)	2.6(8)	N(2)-C(6)-C(7)-C(8)	0.1(6)
C(5)-C(6)-C(7)-C(8)	176.9(5)	C(6)-C(7)-C(8)-C(9)	0.4(6)
C(6)-N(2)-C(9)-C(10)	-177.2(4)	Zn-N(2)-C(9)-C(10)	-12.1(7)
C(6)-N(2)-C(9)-C(8)	0.7(5)	Zn-N(2)-C(9)-C(8)	165.9(3)
C(7)-C(8)-C(9)-N(2)	-0.7(6)	C(7)-C(8)-C(9)-C(10)	177.2(5)
N(2)-C(9)-C(10)-C(11)	3.0(8)	C(8)-C(9)-C(10)-C(11)	-174.6(5)
N(2)-C(9)-C(10)-C(27)	-178.6(4)	C(8)-C(9)-C(10)-C(27)	3.8(7)
C(14)-N(3)-C(11)-C(10)	-179.0(4)	Zn-N(3)-C(11)-C(10)	13.5(7)
C(14)-N(3)-C(11)-C(12)	1.0(5)	Zn-N(3)-C(11)-C(12)	-166.5(3)
C(9)-C(10)-C(11)-N(3)	-3.9(8)	C(27)-C(10)-C(11)-N(3)	177.7(4)
C(9)-C(10)-C(11)-C(12)	176.2(5)	C(27)-C(10)-C(11)-C(12)	-2.3(7)
N(3)-C(11)-C(12)-C(13)	0.4(6)	C(10)-C(11)-C(12)-C(13)	-179.6(5)
C(11)-C(12)-C(13)-C(14)	-1.6(6)	C(11)-N(3)-C(14)-C(15)	173.7(4)
Zn-N(3)-C(14)-C(15)	-18.6(6)	C(11)-N(3)-C(14)-C(13)	-2.0(5)
Zn-N(3)-C(14)-C(13)	165.7(3)	C(12)-C(13)-C(14)-N(3)	2.3(6)
C(12)-C(13)-C(14)-C(15)	-173.4(5)	N(3)-C(14)-C(15)-C(16)	-1.0(7)
C(13)-C(14)-C(15)-C(16)	174.1(5)	N(3)-C(14)-C(15)-C(33)	-178.5(4)
C(13)-C(14)-C(15)-C(33)	-3.4(7)	C(19)-N(4)-C(16)-C(15)	-178.2(5)
Zn-N(4)-C(16)-C(15)	4.8(7)	C(19)-N(4)-C(16)-C(17)	-0.8(5)
Zn-N(4)-C(16)-C(17)	-177.7(3)	C(14)-C(15)-C(16)-N(4)	8.7(8)

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Table S6. concluded for **1D**.

C(33)-C(15)-C(16)-N(4)	-173.8(4)	C(14)-C(15)-C(16)-C(17)	-168.4(4)
C(33)-C(15)-C(16)-C(17)	9.1(7)	N(4)-C(16)-C(17)-C(18)	0.7(6)
C(15)-C(16)-C(17)-C(18)	178.2(5)	C(16)-C(17)-C(18)-C(19)	-0.3(6)
C(16)-N(4)-C(19)-C(20)	179.2(4)	Zn-N(4)-C(19)-C(20)	-3.8(6)
C(16)-N(4)-C(19)-C(18)	0.6(5)	Zn-N(4)-C(19)-C(18)	177.6(3)
C(17)-C(18)-C(19)-N(4)	-0.1(6)	C(17)-C(18)-C(19)-C(20)	-178.8(5)
N(1)-C(1)-C(20)-C(19)	1.7(7)	C(2)-C(1)-C(20)-C(19)	-176.8(4)
N(1)-C(1)-C(20)-C(39)	174.3(4)	C(2)-C(1)-C(20)-C(39)	-4.2(7)
N(4)-C(19)-C(20)-C(1)	-3.3(7)	C(18)-C(19)-C(20)-C(1)	175.1(4)
N(4)-C(19)-C(20)-C(39)	-176.0(4)	C(18)-C(19)-C(20)-C(39)	2.5(6)
C(6)-C(5)-C(21)-C(26)	-80.9(7)	C(4)-C(5)-C(21)-C(26)	96.4(6)
C(6)-C(5)-C(21)-C(22B)	78.1(13)	C(4)-C(5)-C(21)-C(22B)	-104.5(13)
C(6)-C(5)-C(21)-C(22A)	119.4(10)	C(4)-C(5)-C(21)-C(22A)	-63.3(11)
C(26)-C(21)-C(22A)-C(23A)	14(2)	C(5)-C(21)-C(22A)-C(23A)	175.6(10)
C(21)-C(22A)-C(23A)-C(24)	4(2)	C(26)-C(21)-C(22B)-C(23B)	-21(2)
C(5)-C(21)-C(22B)-C(23B)	179.3(12)	C(21)-C(22B)-C(23B)-C(24)	-4(3)
C(22A)-C(23A)-C(24)-C(25)	-21(2)	C(22B)-C(23B)-C(24)-C(25)	26(2)
C(23A)-C(24)-C(25)-C(26)	19(2)	C(23B)-C(24)-C(25)-C(26)	-25(2)
C(22B)-C(21)-C(26)-C(25)	24(2)	C(22A)-C(21)-C(26)-C(25)	-16.2(11)
C(5)-C(21)-C(26)-C(25)	-177.6(5)	C(24)-C(25)-C(26)-C(21)	0.6(11)
C(11)-C(10)-C(27)-C(28B)	50(2)	C(9)-C(10)-C(27)-C(28B)	-128(2)
C(11)-C(10)-C(27)-C(32)	-103.2(6)	C(9)-C(10)-C(27)-C(32)	78.3(7)
C(11)-C(10)-C(27)-C(28A)	87.3(9)	C(9)-C(10)-C(27)-C(28A)	-91.3(9)
C(32)-C(27)-C(28A)-C(29A)	12(2)	C(10)-C(27)-C(28A)-C(29A)	-178.5(9)
C(27)-C(28A)-C(29A)-C(30A)	-1(2)	C(28A)-C(29A)-C(30A)-C(31A)	-4(2)
C(29A)-C(30A)-C(31A)-C(32)	0(3)	C(32)-C(27)-C(28B)-C(29B)	-15(3)
C(10)-C(27)-C(28B)-C(29B)	-172(2)	C(27)-C(28B)-C(29B)-C(30B)	10(4)
C(28B)-C(29B)-C(30B)-C(31B)	-7(5)	C(29B)-C(30B)-C(31B)-C(32)	11(5)
C(28B)-C(27)-C(32)-C(31B)	25(3)	C(10)-C(27)-C(32)-C(31B)	-176(3)
C(28A)-C(27)-C(32)-C(31A)	-16(2)	C(10)-C(27)-C(32)-C(31A)	175.5(11)
C(30B)-C(31B)-C(32)-C(27)	-24(5)	C(30A)-C(31A)-C(32)-C(27)	10(2)
C(14)-C(15)-C(33)-C(38)	-118.3(5)	C(16)-C(15)-C(33)-C(38)	64.1(6)
C(14)-C(15)-C(33)-C(34)	64.9(6)	C(16)-C(15)-C(33)-C(34)	-112.7(5)
C(38)-C(33)-C(34)-C(35)	-0.4(8)	C(15)-C(33)-C(34)-C(35)	176.5(5)
C(33)-C(34)-C(35)-C(36)	-2.1(9)	C(34)-C(35)-C(36)-C(37)	2.7(10)
C(35)-C(36)-C(37)-C(38)	-0.8(10)	C(34)-C(33)-C(38)-C(37)	2.3(8)
C(15)-C(33)-C(38)-C(37)	-174.6(5)	C(36)-C(37)-C(38)-C(33)	-1.7(9)
C(43)-N(5)-C(39)-C(40)	0.8(7)	Zn' -N(5)-C(39)-C(40)	-177.6(4)
C(43)-N(5)-C(39)-C(20)	178.6(4)	Zn' -N(5)-C(39)-C(20)	0.2(6)
C(1)-C(20)-C(39)-N(5)	90.7(5)	C(19)-C(20)-C(39)-N(5)	-95.9(5)
C(1)-C(20)-C(39)-C(40)	-91.4(5)	C(19)-C(20)-C(39)-C(40)	81.9(6)
N(5)-C(39)-C(40)-C(41)	1.6(8)	C(20)-C(39)-C(40)-C(41)	-176.2(5)
C(39)-C(40)-C(41)-C(42)	-2.6(8)	C(40)-C(41)-C(42)-C(43)	1.2(8)
C(39)-N(5)-C(43)-C(42)	-2.3(8)	Zn' -N(5)-C(43)-C(42)	176.4(4)
C(41)-C(42)-C(43)-N(5)	1.3(9)		

Symmetry transformations used to generate equivalent atoms:
' -x,-y+1,-z+1

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Table S7. Weighted least-squares planes, lines and dihedral angles for **1D**.

WEIGHTED LEAST-SQUARES PLANES THROUGH THE STARRED ATOMS
(NARDELLI, MUSATTI, DOMIANO & ANDREETTI, RIC.SCI.(1965),15(II-A),807)
EQUATION OF THE PLANE: M1*X+M2*Y+M3*Z=D

PLANE 1

M1 = 0.50497(0.00033)
M2 = -0.20240(0.00045)
M3 = -0.83907(0.00021)
D = -8.16876(0.00338)

ATOM		D	S	D/S	(D/S)**2
N1	*	-0.1440	0.0040	-36.134	1305.702
N2	*	0.0125	0.0040	3.132	9.812
N3	*	-0.0597	0.0040	-14.819	219.609
N4	*	-0.1102	0.0039	-28.144	792.101
C1	*	0.0046	0.0050	0.922	0.849
C2	*	0.0950	0.0054	17.694	313.060
C3	*	0.0250	0.0056	4.462	19.907
C4	*	-0.1247	0.0053	-23.724	562.807
C5	*	-0.1394	0.0050	-27.933	780.226
C6	*	-0.0587	0.0052	-11.304	127.784
C7	*	0.0373	0.0052	7.125	50.768
C8	*	0.1626	0.0057	28.558	815.539
C9	*	0.1396	0.0050	27.721	768.440
C10	*	0.1893	0.0052	36.172	1308.432
C11	*	0.0631	0.0054	11.784	138.863
C12	*	0.0374	0.0059	6.335	40.139
C13	*	-0.1060	0.0057	-18.446	340.243
C14	*	-0.1352	0.0051	-26.534	704.057
C15	*	-0.1421	0.0050	-28.645	820.513
C16	*	-0.0507	0.0050	-10.137	102.757
C17	*	0.1803	0.0053	33.907	1149.707
C18	*	0.2439	0.0053	45.828	2100.190
C19	*	0.0603	0.0048	12.518	156.694
C20	*	0.0832	0.0047	17.614	310.267
ZN		-0.4818	0.0010	-501.427	251429.000
N5'		-2.6618	0.0040	-673.650	453804.188
					==========
SUM((D/S)**2) FOR STARRED ATOMS					12938.468

CHI-SQUARED AT 95% FOR 21 DEGREES OF FREEDOM: 32.70
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 2

M1 = 0.50497(0.00037)
M2 = -0.20240(0.00042)
M3 = -0.83907(0.00023)
D = -11.47468(0.00150)

ATOM		D	S	D/S	(D/S)**2
N1'	*	0.1440	0.0040	36.135	1305.702
N2'	*	-0.0125	0.0040	-3.132	9.812
N3'	*	0.0597	0.0040	14.819	219.609

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N4' *	0.1102	0.0039	28.144	792.101
C1' *	-0.0046	0.0050	-0.922	0.849
C2' *	-0.0950	0.0054	-17.693	313.060
C3' *	-0.0250	0.0056	-4.462	19.906
C4' *	0.1247	0.0053	23.724	562.807
C5' *	0.1394	0.0050	27.932	780.223
C6' *	0.0587	0.0052	11.304	127.783
C7' *	-0.0373	0.0052	-7.125	50.769
C8' *	-0.1626	0.0057	-28.558	815.535
C9' *	-0.1396	0.0050	-27.721	768.452
C10'*	-0.1893	0.0052	-36.172	1308.416
C11'*	-0.0631	0.0054	-11.784	138.867
C12'*	-0.0374	0.0059	-6.336	40.139
C13'*	0.1060	0.0057	18.446	340.241
C14'*	0.1352	0.0051	26.534	704.061
C15'*	0.1421	0.0050	28.645	820.515
C16'*	0.0507	0.0050	10.137	102.757
C17'*	-0.1803	0.0053	-33.907	1149.706
C18'*	-0.2439	0.0053	-45.828	2100.197
C19'*	-0.0603	0.0048	-12.518	156.695
C20'*	-0.0832	0.0047	-17.614	310.264
ZN'	0.4818	0.0010	501.427	251429.031
N5	2.6618	0.0040	673.650	453804.594
				==========
SUM((D/S)**2) FOR STARRED ATOMS				12938.468

CHI-SQUARED AT 95% FOR 21 DEGREES OF FREEDOM: 32.70
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 3

M1 = 0.48027(0.00125)
M2 = -0.22834(0.00132)
M3 = -0.84688(0.00074)
D = -8.47927(0.00968)

ATOM	D	S	D/S	(D/S)**2
N1 *	-0.0265	0.0040	-6.697	44.854
N2 *	0.0269	0.0040	6.760	45.692
N3 *	-0.0271	0.0040	-6.788	46.073
N4 *	0.0257	0.0039	6.594	43.477
ZN	-0.4062	0.0009	-429.430	184409.984
N5'	-2.5984	0.0039	-660.739	436575.969
N4'	-2.9856	0.0039	-765.269	585637.063
N3'	-2.9327	0.0040	-733.294	537719.938
N2'	-2.9868	0.0040	-750.663	563494.438
N1'	-2.9334	0.0040	-740.985	549059.313
				==========
SUM((D/S)**2) FOR STARRED ATOMS				180.097

CHI-SQUARED AT 95% FOR 1 DEGREES OF FREEDOM: 3.84
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 4

M1 = 0.48027(0.00118)
M2 = -0.22834(0.00135)

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M3 = -0.84688(0.00070)
D = -11.43915(0.00353)

ATOM	D	S	D/S	(D/S)**2
N1' *	0.0265	0.0040	6.697	44.854
N2' *	-0.0269	0.0040	-6.760	45.691
N3' *	0.0271	0.0040	6.788	46.073
N4' *	-0.0257	0.0039	-6.594	43.477
ZN'	0.4062	0.0009	429.430	184409.828
N5	2.5984	0.0039	660.739	436576.281
N4	2.9856	0.0039	765.269	585637.188
N3	2.9327	0.0040	733.294	537720.000
N2	2.9868	0.0040	750.663	563494.813
N1	2.9334	0.0040	740.985	549059.375
				180.095

SUM((D/S)**2) FOR STARRED ATOMS
CHI-SQUARED AT 95% FOR 1 DEGREES OF FREEDOM: 3.84
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 5
M1 = -0.66775(0.00165)
M2 = 0.57608(0.00185)
M3 = -0.47143(0.00195)
D = 2.64938(0.03126)

ATOM	D	S	D/S	(D/S)**2
N5' *	-0.0070	0.0043	-1.645	2.707
C39'*	0.0001	0.0051	0.022	0.000
C40'*	0.0132	0.0060	2.189	4.793
C41'*	-0.0142	0.0063	-2.271	5.157
C42'*	-0.0004	0.0058	-0.074	0.005
C43'*	0.0150	0.0062	2.427	5.892
ZN	-0.0984	0.0012	-81.051	6569.254
N1	-1.6250	0.0043	-381.936	145875.016
N2	-1.5024	0.0044	-343.604	118063.547
N3	1.3787	0.0043	318.590	101499.680
N4	1.2624	0.0042	298.065	88842.617
				18.555

SUM((D/S)**2) FOR STARRED ATOMS
CHI-SQUARED AT 95% FOR 3 DEGREES OF FREEDOM: 7.81
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 6
M1 = -0.66775(0.00180)
M2 = 0.57608(0.00189)
M3 = -0.47143(0.00194)
D = 2.32384(0.01675)

ATOM	D	S	D/S	(D/S)**2
N5 *	0.0070	0.0043	1.645	2.707
C39 *	-0.0001	0.0051	-0.022	0.000
C40 *	-0.0132	0.0060	-2.189	4.793
C41 *	0.0142	0.0063	2.271	5.157
C42 *	0.0004	0.0058	0.073	0.005
C43 *	-0.0150	0.0062	-2.427	5.892

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ZN	0.2271	0.0012	187.045	34985.941
N1	-1.2994	0.0043	-305.422	93282.430
N2	-1.1768	0.0044	-269.151	72442.133
N3	1.7042	0.0043	393.816	155090.781
N4	1.5879	0.0042	374.928	140571.016
				==========
SUM((D/S)**2) FOR STARRED ATOMS				18.554

CHI-SQUARED AT 95% FOR 3 DEGREES OF FREEDOM: 7.81
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

WEIGHTED LEAST-SQUARES LINES THROUGH THE STARRED ATOMS
(SCHOEMAKER,WASER,MARSH & BERGMAN,ACTA CRYST.(1959)12,600
M1,M2,M3 ARE THE DIRECTION COSINES REFERRED TO THE X,Y,Z ORTHOGONAL AXES
X0,Y0,Z0 ARE THE COORDINATES OF THE CENTROID OF THE SET OF ATOMS
EQUATION OF THE LINE:' (X-X0)/M1=(Y-Y0)/M2=(Z-Z0)/M3

LINE 1

M1 = 0.39012(0.00191) X0 = -2.09425(0.00341)
M2 = -0.32465(0.00176) Y0 = 8.80945(0.00304)
M3 = -0.86163(0.00102) Z0 = 8.22338(0.00264)

ATOM	D	S	D/S	(D/S)**2
N5' *	0.0000	0.0061	0.001	0.000
ZN *	0.0000	0.0018	0.002	0.000
N1	1.9989	0.0060	332.277	110407.930
N2	2.0706	0.0062	331.866	110134.922
N3	2.0836	0.0061	340.806	116148.914
N4	1.9528	0.0061	322.410	103948.445
ZN'	5.6866	0.0018	3240.405	10500225.000
N5	5.6866	0.0061	936.893	877769.063
C39'	1.0313	0.0072	143.070	20468.883
C40'	0.8255	0.0085	96.577	9327.148
C41'	0.4671	0.0089	52.716	2778.963
C42'	1.5057	0.0082	182.815	33421.242
C43'	1.2330	0.0087	141.539	20033.271
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

LINE 2

M1 = -0.39012(0.00196) X0 = -5.35453(0.00341)
M2 = 0.32465(0.00183) Y0 = 4.12555(0.00304)
M3 = 0.86163(0.00100) Z0 = 7.58458(0.00264)

ATOM	D	S	D/S	(D/S)**2
N5 *	0.0000	0.0061	0.001	0.000
ZN' *	0.0000	0.0018	0.002	0.000
N1	4.5632	0.0060	758.552	575401.313
N2	7.3132	0.0062	1172.131	1373890.500
N3	7.3367	0.0061	1200.035	1440084.625
N4	4.5891	0.0061	757.688	574091.250
ZN	5.6866	0.0018	3240.406	10500228.000
N5'	5.6866	0.0061	936.893	877768.938
C39	1.0313	0.0072	143.070	20468.926
C40	0.8255	0.0085	96.577	9327.165
C41	0.4671	0.0089	52.716	2778.956

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C42	1.5057	0.0082	182.815	33421.215
C43	1.2330	0.0087	141.539	20033.246
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

LINE 3

M1 = -0.25049(0.00285) X0 = -2.87308(0.00590)
M2 = 0.41925(0.00227) Y0 = 9.74995(0.00503)
M3 = 0.87263(0.00123) Z0 = 10.38654(0.00462)

ATOM	D	S	D/S	(D/S)**2
N5' *	0.0000	0.0061	0.001	0.000
C41'*	0.0000	0.0089	0.001	0.000
ZN	0.3725	0.0018	209.562	43916.059
N1	1.8390	0.0061	302.789	91681.289
N2	2.4166	0.0063	384.944	148181.891
N3	2.3026	0.0062	372.552	138795.125
N4	1.5396	0.0061	253.351	64186.559
ZN'	5.4837	0.0018	3085.283	9518972.000
N5	5.1296	0.0061	840.175	705893.813
C39'	1.1570	0.0073	159.569	25462.406
C40'	1.1711	0.0086	135.925	18475.553
C42'	1.1786	0.0083	142.132	20201.512
C43'	1.1295	0.0088	128.764	16580.139
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

LINE 4

M1 = 0.46798(0.00251) X0 = -2.87289(0.00591)
M2 = 0.81727(0.00152) Y0 = 9.76418(0.00522)
M3 = 0.33625(0.00239) Z0 = 10.38148(0.00478)

ATOM	D	S	D/S	(D/S)**2
C39'*	0.0000	0.0070	0.001	0.000
C42'*	0.0000	0.0080	0.001	0.000
ZN	3.2334	0.0016	2049.910	4202131.500
N1	3.5752	0.0059	607.468	369017.906
N2	4.2252	0.0060	707.600	500697.219
N3	4.2539	0.0060	711.630	506416.906
N4	3.5912	0.0058	619.660	383978.188
ZN'	0.3059	0.0016	193.957	37619.336
N5	1.8742	0.0059	320.247	102557.852
N5'	1.1814	0.0059	201.872	40752.395
C40'	1.1741	0.0083	140.936	19863.074
C41'	1.1901	0.0086	137.599	18933.379
C43'	1.1434	0.0086	133.384	17791.328
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

DIHEDRAL ANGLES FORMED BY LSQ-PLANES

PLANE - PLANE		ANGLE(E.S.D.)
1	2	0.00(0.04)
1	3	2.10(0.08)
1	4	2.10(0.07)
1	5	93.34(0.12)

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1	6	93.34(0.11)
2	3	2.10(0.08)
2	4	2.10(0.07)
2	5	93.34(0.11)
2	6	93.34(0.12)
3	4	0.00(0.13)
3	5	93.04(0.13)
3	6	93.04(0.12)
4	5	93.04(0.13)
4	6	93.04(0.13)
5	6	0.00(0.20)

ANGLES FORMED BY LSQ-LINES

LINE	- LINE	ANGLE(E.S.D.)
1	2	180.00(0.20)
1	3	170.30(0.19)
1	4	111.87(0.17)
2	3	9.70(0.19)
2	4	68.13(0.18)
3	4	58.75(0.21)

ANGLES FORMED BY LINES AND NORMALS TO PLANES

LINE	- PLANE	ANGLE(E.S.D.)
1	1	9.71(0.11)
1	2	9.71(0.11)
1	3	7.61(0.13)
1	4	7.61(0.13)
1	5	92.37(0.15)
1	6	92.37(0.13)
2	1	170.29(0.11)
2	2	170.29(0.11)
2	3	172.39(0.13)
2	4	172.39(0.12)
2	5	87.63(0.14)
2	6	87.63(0.15)
3	1	160.66(0.15)
3	2	160.66(0.15)
3	3	162.76(0.17)
3	4	162.76(0.17)
3	5	90.15(0.16)
3	6	90.15(0.17)
4	1	102.19(0.14)
4	2	102.19(0.14)
4	3	104.28(0.16)
4	4	104.28(0.16)
4	5	90.01(0.18)
4	6	90.01(0.17)

EQUIVALENT POSITIONS:
X,Y,Z
X, 1/2-Y, 1/2+Z
PLUS THE CENTROSYMMETRIC ONES

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Table S8. Crystal data and structure refinement for **3D**.

Empirical formula	$C_{44.5}\ H_{22.5}\ Cl_{4.5}\ F_6\ N_5\ Zn$
Formula weight	966.07
Temperature	153(5) K
Radiation (type, wavelength)	Mo Kα, 0.71073 Å
Diffractometer, Monochromator type	CAD4, graphite
Standard reflections, no. & interval	2, 3600 s
Decay of standards	< 1 %
Crystal system, space group	triclinic, P-1
No. refls, θ range for cell det'n	25, 11.5 to 14.4 °
Unit cell dimensions a = 13.019(5) Å α = 65.14(2) ° b = 13.065(3) Å β = 64.17(2) ° c = 14.908(3) Å γ = 71.36(2) °	
Volume	2041.9(10) Å^3
Z	2
Density (calculated)	1.571 Mg/m^3
Absorption coefficient	0.964 mm^{-1}
F(000)	970
Crystal color, description	red, hexagonal prism
Crystal size	0.25 x 0.10 x 0.05 mm
θ range for data collection	2 to 23 °
Scan type, speeds	ω - 2θ, 1.6 to 5.5 ° min^{-1}
Scan ranges, apertures	1.20 + 0.35*tan*θ, 2.20 + 1.05*tan*θ
Index ranges	-12<=h<=14, -13<=k<=14, 0<=l<=16

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Table S8. concluded for **3D**.

Reflections collected	5552
Absorption correction	Numerical grid
Max. and min. transmission	0.995 and 0.986
Independent reflections	5315 [R(int) = 0.024]
Observed reflections	4655
Refinement method (SHELXL93)	Full-matrix least-squares on F^2
Data / restraints / parameters	5315 / 138 / 606
Goodness-of-fit on F^2	1.048
Final R(F), wR(F^2) [$I>2\sigma(I)$]	0.039 , 0.098
Final R(F), wR(F^2) (all data)	0.048 , 0.102
Largest diff. peak and hole	0.5 and -0.4 e·Å^{-3}

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Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^4) for **3D**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zn(1)	79.9(3)	2497.5(3)	1149.7(3)	200(1)
F(1)	-5960(2)	4403(2)	5346(2)	518(6)
F(2)	-6571(2)	1561(2)	4611(2)	524(6)
F(3)	1332(2)	-2953(2)	5922(2)	522(6)
F(4)	1131(3)	-4465(2)	3686(2)	856(11)
F(5)	5417(2)	-44(2)	-3280(2)	675(8)
F(6)	6240(2)	3241(2)	-3395(2)	565(7)
N(1)	-1451(2)	3619(2)	1137(2)	204(6)
N(2)	-880(2)	1388(2)	2538(2)	218(6)
N(3)	1385(2)	1066(2)	972(2)	215(6)
N(4)	805(2)	3286(2)	-447(2)	208(6)
N(5)	-938(2)	6935(2)	-1799(2)	219(6)
C(1)	-1604(3)	4579(3)	313(2)	225(7)
C(2)	-2781(3)	5174(3)	629(3)	270(7)
C(3)	-3332(3)	4554(3)	1626(3)	272(8)
C(4)	-2503(3)	3571(3)	1938(3)	221(7)
C(5)	-2769(3)	2656(3)	2887(2)	224(7)
C(6)	-2013(3)	1634(3)	3145(2)	219(7)
C(7)	-2327(3)	669(3)	4090(3)	291(8)
C(8)	-1390(3)	-159(3)	4034(3)	269(8)
C(9)	-482(3)	283(3)	3071(2)	225(7)
C(10)	622(3)	-343(3)	2715(2)	228(7)
C(11)	1490(3)	32(3)	1747(3)	231(7)
C(12)	2642(3)	-594(3)	1401(3)	281(8)
C(13)	3210(3)	51(3)	429(3)	273(8)
C(14)	2416(3)	1087(3)	146(3)	233(7)
C(15)	2648(3)	1955(3)	-843(3)	243(8)
C(16)	1864(3)	2960(3)	-1113(2)	229(7)
C(17)	2060(3)	3778(3)	-2166(3)	285(8)
C(18)	1110(3)	4583(3)	-2121(3)	277(8)
C(19)	325(3)	4284(3)	-1053(2)	222(7)
C(20)	-783(3)	4902(3)	-694(2)	207(7)
C(21)	-3995(3)	2758(3)	3641(2)	238(8)
C(22)	-4414(3)	3548(3)	4167(3)	292(8)
C(23)	-5549(3)	3632(3)	4832(3)	315(7)
C(24)	-6298(3)	2975(3)	5011(3)	346(9)
C(25)	-5851(3)	2207(3)	4471(3)	330(9)
C(26)	-4733(3)	2080(3)	3797(3)	291(8)
C(27)	861(3)	-1529(3)	3440(3)	245(8)
C(28)	999(3)	-1705(3)	4367(3)	261(8)
C(29)	1180(3)	-2800(3)	5033(3)	302(8)
C(30)	1218(3)	-3745(3)	4836(3)	372(9)

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Table S9. concluded for **3D**.

C(31)	1086(4)	-3545(3)	3914(3)	448(11)
C(32)	918(4)	-2470(3)	3204(3)	376(9)
C(33)	3785(3)	1795(3)	-1692(3)	267(8)
C(34)	4096(3)	902(3)	-2080(3)	356(9)
C(35)	5121(3)	826(3)	-2898(3)	402(10)
C(36)	5866(3)	1593(3)	-3366(3)	400(10)
C(37)	5536(3)	2459(3)	-2961(3)	364(9)
C(38)	4529(3)	2581(3)	-2139(3)	299(8)
C(39)	-1181(3)	5892(3)	-1520(2)	227(7)
C(40)	-1794(3)	5711(3)	-1982(3)	370(9)
C(41)	-2183(3)	6597(3)	-2740(3)	392(9)
C(42)	-1944(3)	7663(3)	-3019(3)	284(8)
C(43)	-1322(3)	7787(3)	-2548(3)	284(8)
C(44A)	4251(10)	7500(9)	-143(9)	662(31)
Cl(1A)	3873(6)	6433(6)	1179(4)	540(14)
Cl(2A)	5549(2)	7969(2)	-555(2)	514(9)
Cl(3A)	4246(5)	7000(5)	-1033(5)	1366(21)
C(44B)	3860(10)	6721(10)	-49(9)	834(33)
Cl(1B)	3945(8)	6266(7)	1141(7)	1302(32)
Cl(2B)	2608(3)	7647(3)	-171(3)	1075(14)
Cl(3B)	5068(4)	7393(5)	-950(3)	1611(28)
C(45)	154(11)	9526(12)	-20(13)	846(45)
Cl(4)	-837(6)	9627(6)	1188(6)	976(19)
Cl(5)	1309(4)	8438(5)	44(5)	1434(24)
Cl(6)	529(7)	10821(7)	-913(6)	1198(25)

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Table S10. Bond lengths [Å] and angles [°] for **3D**.

Zn(1)-N(4)	2.055(3)	Zn(1)-N(1)	2.065(3)
Zn(1)-N(2)	2.081(3)	Zn(1)-N(3)	2.109(3)
Zn(1)-N(5)'	2.193(3)	F(1)-C(23)	1.354(4)
F(2)-C(25)	1.349(4)	F(3)-C(29)	1.348(4)
F(4)-C(31)	1.357(4)	F(5)-C(35)	1.355(4)
F(6)-C(37)	1.352(4)	N(1)-C(4)	1.369(4)
N(1)-C(1)	1.371(4)	N(2)-C(6)	1.370(4)
N(2)-C(9)	1.378(4)	N(3)-C(14)	1.369(4)
N(3)-C(11)	1.373(4)	N(4)-C(16)	1.362(4)
N(4)-C(19)	1.373(4)	N(5)-C(39)	1.346(4)
N(5)-C(43)	1.350(4)	N(5)-Zn(1)'	2.193(3)
C(1)-C(20)	1.391(5)	C(1)-C(2)	1.446(5)
C(2)-C(3)	1.346(5)	C(3)-C(4)	1.441(5)
C(4)-C(5)	1.403(5)	C(5)-C(6)	1.399(5)
C(5)-C(21)	1.502(5)	C(6)-C(7)	1.441(5)
C(7)-C(8)	1.345(5)	C(8)-C(9)	1.433(5)
C(9)-C(10)	1.402(5)	C(10)-C(11)	1.392(5)
C(10)-C(27)	1.498(4)	C(11)-C(12)	1.442(5)
C(12)-C(13)	1.339(5)	C(13)-C(14)	1.443(5)
C(14)-C(15)	1.406(5)	C(15)-C(16)	1.408(5)
C(15)-C(33)	1.493(5)	C(16)-C(17)	1.445(5)
C(17)-C(18)	1.341(5)	C(18)-C(19)	1.432(5)
C(19)-C(20)	1.401(5)	C(20)-C(39)	1.499(4)
C(21)-C(22)	1.388(5)	C(21)-C(26)	1.392(5)
C(22)-C(23)	1.375(5)	C(23)-C(24)	1.369(5)
C(24)-C(25)	1.374(5)	C(25)-C(26)	1.367(5)
C(27)-C(28)	1.385(5)	C(27)-C(32)	1.388(5)
C(28)-C(29)	1.371(5)	C(29)-C(30)	1.367(5)
C(30)-C(31)	1.366(6)	C(31)-C(32)	1.377(5)
C(33)-C(34)	1.387(5)	C(33)-C(38)	1.392(5)
C(34)-C(35)	1.370(5)	C(35)-C(36)	1.370(6)
C(36)-C(37)	1.366(5)	C(37)-C(38)	1.370(5)
C(39)-C(40)	1.379(5)	C(40)-C(41)	1.378(5)
C(41)-C(42)	1.374(5)	C(42)-C(43)	1.361(5)
C(44A)-Cl(3A)	1.709(11)	C(44A)-Cl(2A)	1.747(12)
C(44A)-Cl(1A)	1.832(13)	C(44B)-Cl(1B)	1.659(13)
C(44B)-Cl(2B)	1.722(10)	C(44B)-Cl(3B)	1.760(13)
Cl(2B)-Cl(5)	1.649(5)	C(45)-Cl(5)	1.714(13)
C(45)-Cl(6)	1.71(2)	C(45)-Cl(4)	1.73(2)

N(4)-Zn(1)-N(1)	89.4(1)	N(4)-Zn(1)-N(2)	157.67(1)
N(1)-Zn(1)-N(2)	87.8(1)	N(4)-Zn(1)-N(3)	87.5(1)
N(1)-Zn(1)-N(3)	159.1(1)	N(2)-Zn(1)-N(3)	87.2(1)
N(4)-Zn(1)-N(5)'	102.5(1)	N(1)-Zn(1)-N(5)'	107.6(1)
N(2)-Zn(1)-N(5)'	99.4(1)	N(3)-Zn(1)-N(5)'	93.3(1)

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Table S10. continued for **3D**.

C(4)-N(1)-C(1)	106.3(3)	C(4)-N(1)-Zn(1)	127.6(2)
C(1)-N(1)-Zn(1)	126.1(2)	C(6)-N(2)-C(9)	106.1(3)
C(6)-N(2)-Zn(1)	126.9(2)	C(9)-N(2)-Zn(1)	126.9(2)
C(14)-N(3)-C(11)	106.7(3)	C(14)-N(3)-Zn(1)	125.3(2)
C(11)-N(3)-Zn(1)	126.4(2)	C(16)-N(4)-C(19)	106.0(3)
C(16)-N(4)-Zn(1)	127.6(2)	C(19)-N(4)-Zn(1)	126.3(2)
C(39)-N(5)-C(43)	116.9(3)	C(39)-N(5)-Zn(1)'	129.5(2)
C(43)-N(5)-Zn(1)'	113.5(2)	N(1)-C(1)-C(20)	125.6(3)
N(1)-C(1)-C(2)	109.6(3)	C(20)-C(1)-C(2)	124.7(3)
C(3)-C(2)-C(1)	107.1(3)	C(2)-C(3)-C(4)	106.9(3)
N(1)-C(4)-C(5)	125.2(3)	N(1)-C(4)-C(3)	110.0(3)
C(5)-C(4)-C(3)	124.5(3)	C(6)-C(5)-C(4)	125.3(3)
C(6)-C(5)-C(21)	118.0(3)	C(4)-C(5)-C(21)	116.5(3)
N(2)-C(6)-C(5)	125.6(3)	N(2)-C(6)-C(7)	109.8(3)
C(5)-C(6)-C(7)	124.5(3)	C(8)-C(7)-C(6)	106.9(3)
C(7)-C(8)-C(9)	107.5(3)	N(2)-C(9)-C(10)	125.8(3)
N(2)-C(9)-C(8)	109.6(3)	C(10)-C(9)-C(8)	124.5(3)
C(11)-C(10)-C(9)	125.8(3)	C(11)-C(10)-C(27)	118.0(3)
C(9)-C(10)-C(27)	116.2(3)	N(3)-C(11)-C(10)	125.1(3)
N(3)-C(11)-C(12)	109.2(3)	C(10)-C(11)-C(12)	125.7(3)
C(13)-C(12)-C(11)	107.5(3)	C(12)-C(13)-C(14)	107.2(3)
N(3)-C(14)-C(15)	125.3(3)	N(3)-C(14)-C(13)	109.4(3)
C(15)-C(14)-C(13)	125.2(3)	C(14)-C(15)-C(16)	124.7(3)
C(14)-C(15)-C(33)	118.5(3)	C(16)-C(15)-C(33)	116.8(3)
N(4)-C(16)-C(15)	125.9(3)	N(4)-C(16)-C(17)	110.0(3)
C(15)-C(16)-C(17)	124.0(3)	C(18)-C(17)-C(16)	106.7(3)
C(17)-C(18)-C(19)	107.4(3)	N(4)-C(19)-C(20)	125.5(3)
N(4)-C(19)-C(18)	109.8(3)	C(20)-C(19)-C(18)	124.6(3)
C(1)-C(20)-C(19)	126.0(3)	C(1)-C(20)-C(39)	116.9(3)
C(19)-C(20)-C(39)	116.3(3)	C(22)-C(21)-C(26)	119.3(3)
C(22)-C(21)-C(5)	120.6(3)	C(26)-C(21)-C(5)	120.1(3)
C(23)-C(22)-C(21)	118.7(3)	F(1)-C(23)-C(24)	117.6(3)
F(1)-C(23)-C(22)	118.8(3)	C(24)-C(23)-C(22)	123.6(3)
C(23)-C(24)-C(25)	115.9(3)	F(2)-C(25)-C(26)	118.9(3)
F(2)-C(25)-C(24)	117.5(3)	C(26)-C(25)-C(24)	123.6(3)
C(25)-C(26)-C(21)	118.9(3)	C(28)-C(27)-C(32)	118.9(3)
C(28)-C(27)-C(10)	120.8(3)	C(32)-C(27)-C(10)	120.2(3)
C(29)-C(28)-C(27)	119.6(3)	F(3)-C(29)-C(30)	118.3(3)
F(3)-C(29)-C(28)	118.6(3)	C(30)-C(29)-C(28)	123.1(3)
C(31)-C(30)-C(29)	116.0(3)	F(4)-C(31)-C(30)	117.6(3)
F(4)-C(31)-C(32)	118.5(4)	C(30)-C(31)-C(32)	123.9(4)
C(31)-C(32)-C(27)	118.5(3)	C(34)-C(33)-C(38)	119.0(3)
C(34)-C(33)-C(15)	121.2(3)	C(38)-C(33)-C(15)	119.8(3)
C(35)-C(34)-C(33)	119.0(4)	F(5)-C(35)-C(36)	117.7(3)
F(5)-C(35)-C(34)	118.7(4)	C(36)-C(35)-C(34)	123.6(4)
C(37)-C(36)-C(35)	115.9(3)	F(6)-C(37)-C(36)	118.2(3)
F(6)-C(37)-C(38)	118.1(3)	C(36)-C(37)-C(38)	123.7(4)
C(37)-C(38)-C(33)	118.9(3)	N(5)-C(39)-C(40)	121.3(3)
N(5)-C(39)-C(20)	120.0(3)	C(40)-C(39)-C(20)	118.7(3)
C(41)-C(40)-C(39)	120.8(3)	C(42)-C(41)-C(40)	118.0(3)
C(43)-C(42)-C(41)	118.6(3)	N(5)-C(43)-C(42)	124.5(3)

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Table S10. concluded for **3D**.

Cl(3A)-C(44A)-Cl(2A)	111.6(7)	Cl(3A)-C(44A)-Cl(1A)	110.2(7)
Cl(2A)-C(44A)-Cl(1A)	113.8(6)	Cl(1B)-C(44B)-Cl(2B)	114.6(7)
Cl(1B)-C(44B)-Cl(3B)	107.1(7)	Cl(2B)-C(44B)-Cl(3B)	109.8(6)
Cl(5)-C(45)-Cl(6)	114.0(9)	Cl(5)-C(45)-Cl(4)	114.9(10)
Cl(6)-C(45)-Cl(4)	112.7(7)		

Symmetry transformations used to generate equivalent atoms:
' -x,-y+1,-z

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Table S11. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3D**. 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
Zn(1)	20.3(2)	16.5(2)	17.4(2)	-2.9(2)	-5.3(2)	-1.4(2)
F(1)	42(1)	54(2)	51(1)	-37(1)	14(1)	-14(1)
F(2)	33(1)	58(2)	69(2)	-28(1)	-4(1)	-21(1)
F(3)	86(2)	35(1)	37(1)	6(1)	-38(1)	-11(1)
F(4)	179(3)	23(1)	65(2)	-10(1)	-57(2)	-14(2)
F(5)	69(2)	64(2)	59(2)	-45(2)	9(1)	-8(1)
F(6)	31(1)	61(2)	57(2)	-17(1)	8(1)	-20(1)
N(1)	20(2)	19(1)	18(1)	-4(1)	-6(1)	-2(1)
N(2)	21(2)	18(1)	19(1)	-4(1)	-4(1)	0(1)
N(3)	20(2)	19(1)	19(1)	-4(1)	-4(1)	-1(1)
N(4)	21(2)	16(1)	20(1)	-5(1)	-5(1)	-1(1)
N(5)	24(2)	18(1)	18(1)	-4(1)	-7(1)	-1(1)
C(1)	26(2)	17(2)	24(2)	-5(1)	-12(2)	-1(1)
C(2)	28(2)	18(2)	28(2)	-3(2)	-13(2)	3(1)
C(3)	20(2)	24(2)	29(2)	-9(2)	-5(2)	2(1)
C(4)	22(2)	19(2)	25(2)	-8(1)	-8(2)	-2(1)
C(5)	23(2)	22(2)	22(2)	-9(1)	-6(1)	-4(1)
C(6)	23(2)	22(2)	18(2)	-6(1)	-4(1)	-5(1)
C(7)	24(2)	30(2)	25(2)	-9(2)	-1(2)	-6(2)
C(8)	28(2)	19(2)	24(2)	-2(1)	-6(2)	-3(2)
C(9)	28(2)	16(2)	17(2)	-3(1)	-5(2)	-3(1)
C(10)	26(2)	17(2)	21(2)	-5(1)	-9(2)	0(1)
C(11)	25(2)	17(2)	23(2)	-5(1)	-8(2)	-2(1)
C(12)	28(2)	21(2)	27(2)	-5(2)	-11(2)	2(2)
C(13)	19(2)	27(2)	26(2)	-9(2)	-5(2)	4(1)
C(14)	21(2)	21(2)	23(2)	-7(1)	-5(2)	-1(1)
C(15)	24(2)	22(2)	21(2)	-5(2)	-5(2)	-4(1)
C(16)	24(2)	20(2)	19(2)	-4(1)	-5(2)	-4(1)
C(17)	27(2)	29(2)	19(2)	-6(2)	-2(2)	-2(2)
C(18)	31(2)	25(2)	16(2)	0(1)	-7(2)	-4(2)
C(19)	29(2)	16(2)	19(2)	-2(1)	-9(2)	-4(1)
C(20)	27(2)	15(2)	21(2)	-4(1)	-11(2)	-3(1)
C(21)	24(2)	18(2)	22(2)	-3(1)	-6(2)	-2(1)
C(22)	27(2)	29(2)	26(2)	-8(2)	0(2)	-10(2)
C(23)	33(2)	30(2)	26(2)	-14(2)	-1(2)	-5(2)
C(24)	21(2)	40(2)	33(2)	-10(2)	0(2)	-3(2)
C(25)	25(2)	32(2)	38(2)	-8(2)	-8(2)	-10(2)
C(26)	28(2)	28(2)	31(2)	-13(2)	-7(2)	-4(2)
C(27)	21(2)	19(2)	23(2)	-4(1)	-3(2)	-1(1)
C(28)	28(2)	21(2)	26(2)	-5(2)	-9(2)	-4(2)
C(29)	29(2)	29(2)	23(2)	0(2)	-9(2)	-5(2)
C(30)	44(2)	19(2)	29(2)	3(2)	-10(2)	-1(2)

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Table S11. concluded for **3D**.

C(31)	75(3)	16(2)	41(2)	-9(2)	-20(2)	-5(2)
C(32)	57(3)	24(2)	29(2)	-6(2)	-17(2)	-4(2)
C(33)	24(2)	26(2)	19(2)	-4(2)	-5(2)	2(2)
C(34)	38(2)	31(2)	27(2)	-9(2)	-1(2)	-6(2)
C(35)	41(2)	38(2)	32(2)	-18(2)	-3(2)	2(2)
C(36)	25(2)	50(3)	27(2)	-13(2)	0(2)	3(2)
C(37)	27(2)	37(2)	31(2)	-3(2)	-5(2)	-6(2)
C(38)	24(2)	27(2)	29(2)	-8(2)	-5(2)	-1(2)
C(39)	24(2)	22(2)	19(2)	-6(1)	-7(1)	-1(1)
C(40)	51(2)	26(2)	42(2)	-2(2)	-28(2)	-12(2)
C(41)	52(3)	34(2)	43(2)	-6(2)	-32(2)	-7(2)
C(42)	33(2)	27(2)	21(2)	-4(2)	-14(2)	1(2)
C(43)	37(2)	19(2)	25(2)	0(2)	-14(2)	-4(2)
C(44A)	73(8)	49(6)	91(9)	-26(6)	-45(7)	0(5)
Cl(1A)	49(3)	57(2)	63(3)	-35(2)	-17(2)	1(2)
Cl(2A)	41(1)	40(1)	60(2)	-16(1)	-19(1)	11(1)
Cl(3A)	156(5)	181(5)	149(5)	-104(4)	-77(4)	-21(4)
C(44B)	100(8)	73(7)	96(8)	-48(6)	-53(7)	16(6)
Cl(1B)	93(5)	119(5)	167(6)	3(4)	-81(4)	-21(4)
Cl(2B)	111(3)	103(2)	176(4)	-82(2)	-107(3)	30(2)
Cl(3B)	86(3)	221(6)	91(3)	-15(3)	-12(2)	4(3)
C(45)	49(8)	126(14)	110(11)	-69(11)	-31(8)	-8(9)
Cl(4)	99(4)	113(5)	118(4)	-64(3)	-57(3)	-2(3)
Cl(5)	87(3)	167(5)	248(6)	-138(5)	-90(4)	31(3)
Cl(6)	131(6)	140(6)	137(6)	-44(4)	-83(5)	-35(5)

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Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **3D**.

	x	y	z	U(eq)
H(2)	-3098(3)	5857(3)	220(3)	32
H(3)	-4101(3)	4726(3)	2036(3)	33
H(7)	-3041(3)	626(3)	4635(3)	35
H(8)	-1340(3)	-885(3)	4531(3)	32
H(12)	2937(3)	-1313(3)	1783(3)	34
H(13)	3973(3)	-134(3)	14(3)	33
H(17)	2718(3)	3750(3)	-2760(3)	34
H(18)	984(3)	5220(3)	-2682(3)	33
H(22)	-3937(3)	4012(3)	4071(3)	35
H(24)	-7061(3)	3044(3)	5469(3)	42
H(26)	-4469(3)	1548(3)	3449(3)	35
H(28)	970(3)	-1086(3)	4537(3)	31
H(30)	1328(3)	-4481(3)	5302(3)	45
H(32)	844(4)	-2377(3)	2580(3)	45
H(34)	3615(3)	362(3)	-1790(3)	43
H(36)	6555(3)	1529(3)	-3925(3)	48
H(38)	4346(3)	3180(3)	-1884(3)	36
H(40)	-1946(3)	4981(3)	-1778(3)	44
H(41)	-2595(3)	6477(3)	-3054(3)	47
H(42)	-2202(3)	8286(3)	-3519(3)	34
H(43)	-1149(3)	8509(3)	-2756(3)	34
H(44A)	3636(10)	8169(9)	-117(9)	79
H(44B)	3916(10)	6054(10)	-220(9)	100
H(45)	-270(11)	9318(12)	-307(13)	102

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Table S13. Torsion angles [°] for **3D**.

N(4)-Zn(1)-N(1)-C(4)	170.5(3)	N(2)-Zn(1)-N(1)-C(4)	12.7(3)
N(3)-Zn(1)-N(1)-C(4)	89.1(4)	N(5)' -Zn(1)-N(1)-C(4)	-86.5(3)
N(4)-Zn(1)-N(1)-C(1)	-10.5(3)	N(2)-Zn(1)-N(1)-C(1)	-168.3(3)
N(3)-Zn(1)-N(1)-C(1)	-91.9(4)	N(5)' -Zn(1)-N(1)-C(1)	92.5(3)
N(4)-Zn(1)-N(2)-C(6)	-94.7(3)	N(1)-Zn(1)-N(2)-C(6)	-11.6(3)
N(3)-Zn(1)-N(2)-C(6)	-171.3(3)	N(5)' -Zn(1)-N(2)-C(6)	95.8(3)
N(4)-Zn(1)-N(2)-C(9)	90.3(4)	N(1)-Zn(1)-N(2)-C(9)	173.4(3)
N(3)-Zn(1)-N(2)-C(9)	13.7(3)	N(5)' -Zn(1)-N(2)-C(9)	-79.2(3)
N(4)-Zn(1)-N(3)-C(14)	20.6(3)	N(1)-Zn(1)-N(3)-C(14)	102.4(3)
N(2)-Zn(1)-N(3)-C(14)	178.9(3)	N(5)' -Zn(1)-N(3)-C(14)	-81.8(3)
N(4)-Zn(1)-N(3)-C(11)	-175.9(3)	N(1)-Zn(1)-N(3)-C(11)	-94.2(4)
N(2)-Zn(1)-N(3)-C(11)	-17.7(3)	N(5)' -Zn(1)-N(3)-C(11)	81.6(3)
N(1)-Zn(1)-N(4)-C(16)	-173.4(3)	N(2)-Zn(1)-N(4)-C(16)	-90.7(4)
N(3)-Zn(1)-N(4)-C(16)	-14.1(3)	N(5)' -Zn(1)-N(4)-C(16)	78.7(3)
N(1)-Zn(1)-N(4)-C(19)	9.3(3)	N(2)-Zn(1)-N(4)-C(19)	92.0(3)
N(3)-Zn(1)-N(4)-C(19)	168.6(3)	N(5)' -Zn(1)-N(4)-C(19)	-98.6(3)
C(4)-N(1)-C(1)-C(20)	-173.9(3)	Zn(1)-N(1)-C(1)-C(20)	6.9(5)
C(4)-N(1)-C(1)-C(2)	2.4(4)	Zn(1)-N(1)-C(1)-C(2)	-176.7(2)
N(1)-C(1)-C(2)-C(3)	-1.6(4)	C(20)-C(1)-C(2)-C(3)	174.8(3)
C(1)-C(2)-C(3)-C(4)	0.1(4)	C(1)-N(1)-C(4)-C(5)	172.4(3)
Zn(1)-N(1)-C(4)-C(5)	-8.5(5)	C(1)-N(1)-C(4)-C(3)	-2.4(4)
Zn(1)-N(1)-C(4)-C(3)	176.8(2)	C(2)-C(3)-C(4)-N(1)	1.4(4)
C(2)-C(3)-C(4)-C(5)	-173.4(3)	N(1)-C(4)-C(5)-C(6)	-2.4(5)
C(3)-C(4)-C(5)-C(6)	171.6(3)	N(1)-C(4)-C(5)-C(21)	-177.4(3)
C(3)-C(4)-C(5)-C(21)	-3.4(5)	C(9)-N(2)-C(6)-C(5)	-177.7(3)
Zn(1)-N(2)-C(6)-C(5)	6.4(5)	C(9)-N(2)-C(6)-C(7)	1.0(4)
Zn(1)-N(2)-C(6)-C(7)	-174.8(2)	C(4)-C(5)-C(6)-N(2)	3.4(5)
C(21)-C(5)-C(6)-N(2)	178.3(3)	C(4)-C(5)-C(6)-C(7)	-175.2(3)
C(21)-C(5)-C(6)-C(7)	-0.3(5)	N(2)-C(6)-C(7)-C(8)	-1.3(4)
C(5)-C(6)-C(7)-C(8)	177.5(3)	C(6)-C(7)-C(8)-C(9)	0.9(4)
C(6)-N(2)-C(9)-C(10)	176.9(3)	Zn(1)-N(2)-C(9)-C(10)	-7.3(5)
C(6)-N(2)-C(9)-C(8)	-0.5(4)	Zn(1)-N(2)-C(9)-C(8)	175.4(2)
C(7)-C(8)-C(9)-N(2)	-0.3(4)	C(7)-C(8)-C(9)-C(10)	-177.7(3)
N(2)-C(9)-C(10)-C(11)	-2.2(6)	C(8)-C(9)-C(10)-C(11)	174.7(3)
N(2)-C(9)-C(10)-C(27)	179.4(3)	C(8)-C(9)-C(10)-C(27)	-3.7(5)
C(14)-N(3)-C(11)-C(10)	-178.5(3)	Zn(1)-N(3)-C(11)-C(10)	15.5(5)
C(14)-N(3)-C(11)-C(12)	2.0(4)	Zn(1)-N(3)-C(11)-C(12)	-163.9(2)
C(9)-C(10)-C(11)-N(3)	-2.3(6)	C(27)-C(10)-C(11)-N(3)	176.1(3)
C(9)-C(10)-C(11)-C(12)	177.1(3)	C(27)-C(10)-C(11)-C(12)	-4.5(5)
N(3)-C(11)-C(12)-C(13)	-0.8(4)	C(10)-C(11)-C(12)-C(13)	179.7(3)
C(11)-C(12)-C(13)-C(14)	-0.6(4)	C(11)-N(3)-C(14)-C(15)	174.7(3)
Zn(1)-N(3)-C(14)-C(15)	-19.1(5)	C(11)-N(3)-C(14)-C(13)	-2.4(4)
Zn(1)-N(3)-C(14)-C(13)	163.8(2)	C(12)-C(13)-C(14)-N(3)	1.9(4)
C(12)-C(13)-C(14)-C(15)	-175.2(3)	N(3)-C(14)-C(15)-C(16)	2.9(6)
C(13)-C(14)-C(15)-C(16)	179.6(3)	N(3)-C(14)-C(15)-C(33)	-174.5(3)
C(13)-C(14)-C(15)-C(33)	2.2(5)	C(19)-N(4)-C(16)-C(15)	-177.3(3)
Zn(1)-N(4)-C(16)-C(15)	5.0(5)	C(19)-N(4)-C(16)-C(17)	0.2(4)
Zn(1)-N(4)-C(16)-C(17)	-177.5(2)	C(14)-C(15)-C(16)-N(4)	5.0(6)

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Table S13. concluded for **3D**.

C(33)-C(15)-C(16)-N(4)	-177.5(3)	C(14)-C(15)-C(16)-C(17)	-172.2(3)
C(33)-C(15)-C(16)-C(17)	5.2(5)	N(4)-C(16)-C(17)-C(18)	-0.4(4)
C(15)-C(16)-C(17)-C(18)	177.2(3)	C(16)-C(17)-C(18)-C(19)	0.3(4)
C(16)-N(4)-C(19)-C(20)	177.9(3)	Zn(1)-N(4)-C(19)-C(20)	-4.4(5)
C(16)-N(4)-C(19)-C(18)	0.0(4)	Zn(1)-N(4)-C(19)-C(18)	177.7(2)
C(17)-C(18)-C(19)-N(4)	-0.2(4)	C(17)-C(18)-C(19)-C(20)	-178.1(3)
N(1)-C(1)-C(20)-C(19)	2.5(5)	C(2)-C(1)-C(20)-C(19)	-173.3(3)
N(1)-C(1)-C(20)-C(39)	171.6(3)	C(2)-C(1)-C(20)-C(39)	-4.2(5)
N(4)-C(19)-C(20)-C(1)	-3.9(5)	C(18)-C(19)-C(20)-C(1)	173.7(3)
N(4)-C(19)-C(20)-C(39)	-173.1(3)	C(18)-C(19)-C(20)-C(39)	4.5(5)
C(6)-C(5)-C(21)-C(22)	114.9(4)	C(4)-C(5)-C(21)-C(22)	-69.8(4)
C(6)-C(5)-C(21)-C(26)	-66.9(4)	C(4)-C(5)-C(21)-C(26)	108.5(4)
C(26)-C(21)-C(22)-C(23)	0.3(5)	C(5)-C(21)-C(22)-C(23)	178.5(3)
C(21)-C(22)-C(23)-F(1)	180.0(3)	C(21)-C(22)-C(23)-C(24)	0.2(6)
F(1)-C(23)-C(24)-C(25)	179.7(3)	C(22)-C(23)-C(24)-C(25)	-0.5(6)
C(23)-C(24)-C(25)-F(2)	-178.6(3)	C(23)-C(24)-C(25)-C(26)	0.4(6)
F(2)-C(25)-C(26)-C(21)	179.1(3)	C(24)-C(25)-C(26)-C(21)	0.0(6)
C(22)-C(21)-C(26)-C(25)	-0.4(5)	C(5)-C(21)-C(26)-C(25)	-178.6(3)
C(11)-C(10)-C(27)-C(28)	110.1(4)	C(9)-C(10)-C(27)-C(28)	-71.3(4)
C(11)-C(10)-C(27)-C(32)	-71.6(4)	C(9)-C(10)-C(27)-C(32)	107.0(4)
C(32)-C(27)-C(28)-C(29)	-0.5(5)	C(10)-C(27)-C(28)-C(29)	177.9(3)
C(27)-C(28)-C(29)-F(3)	178.9(3)	C(27)-C(28)-C(29)-C(30)	-0.8(5)
F(3)-C(29)-C(30)-C(31)	-178.6(3)	C(28)-C(29)-C(30)-C(31)	1.2(6)
C(29)-C(30)-C(31)-F(4)	179.3(4)	C(29)-C(30)-C(31)-C(32)	-0.2(7)
F(4)-C(31)-C(32)-C(27)	179.4(4)	C(30)-C(31)-C(32)-C(27)	-1.0(7)
C(28)-C(27)-C(32)-C(31)	1.4(6)	C(10)-C(27)-C(32)-C(31)	-177.0(4)
C(14)-C(15)-C(33)-C(34)	62.2(5)	C(16)-C(15)-C(33)-C(34)	-115.5(4)
C(14)-C(15)-C(33)-C(38)	-120.8(4)	C(16)-C(15)-C(33)-C(38)	61.6(4)
C(38)-C(33)-C(34)-C(35)	-0.5(5)	C(15)-C(33)-C(34)-C(35)	176.5(3)
C(33)-C(34)-C(35)-F(5)	-179.5(3)	C(33)-C(34)-C(35)-C(36)	-0.3(6)
F(5)-C(35)-C(36)-C(37)	179.8(4)	C(34)-C(35)-C(36)-C(37)	0.6(6)
C(35)-C(36)-C(37)-F(6)	-179.9(3)	C(35)-C(36)-C(37)-C(38)	0.0(6)
F(6)-C(37)-C(38)-C(33)	179.1(3)	C(36)-C(37)-C(38)-C(33)	-0.8(6)
C(34)-C(33)-C(38)-C(37)	1.1(5)	C(15)-C(33)-C(38)-C(37)	-176.0(3)
C(43)-N(5)-C(39)-C(40)	0.0(5)	Zn(1)' -N(5)-C(39)-C(40)	176.1(3)
C(43)-N(5)-C(39)-C(20)	180.0(3)	Zn(1)' -N(5)-C(39)-C(20)	-4.0(4)
C(1)-C(20)-C(39)-N(5)	101.5(4)	C(19)-C(20)-C(39)-N(5)	-88.3(4)
C(1)-C(20)-C(39)-C(40)	-78.6(4)	C(19)-C(20)-C(39)-C(40)	91.6(4)
N(5)-C(39)-C(40)-C(41)	-0.4(6)	C(20)-C(39)-C(40)-C(41)	179.6(4)
C(39)-C(40)-C(41)-C(42)	-0.1(6)	C(40)-C(41)-C(42)-C(43)	1.1(6)
C(39)-N(5)-C(43)-C(42)	1.0(5)	Zn(1)' -N(5)-C(43)-C(42)	-175.7(3)
C(41)-C(42)-C(43)-N(5)	-1.6(5)		

Symmetry transformations used to generate equivalent atoms:
' -x,-y+1,-z

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Table S14. Weighted least-squares planes, lines and dihedral angles for **3D**.

WEIGHTED LEAST-SQUARES PLANES THROUGH THE STARRED ATOMS
(NARDELLI, MUSATTI, DOMIANO & ANDREETTI, RIC.SCI.(1965),15(II-A),807)
EQUATION OF THE PLANE: M1*X+M2*Y+M3*Z=D

PLANE 1

M1 = -0.72647(0.00024)
M2 = -0.58804(0.00028)
M3 = -0.35560(0.00031)
D = -3.50821(0.00100)

ATOM	D	S	D/S	(D/S)**2
N1 *	-0.1957	0.0035	-55.394	3068.481
N2 *	-0.0917	0.0035	-25.954	673.602
N3 *	-0.0508	0.0036	-14.240	202.775
N4 *	-0.1129	0.0035	-31.957	1021.274
C1 *	-0.0668	0.0042	-15.854	251.338
C2 *	0.0591	0.0044	13.505	182.387
C3 *	0.0401	0.0044	9.099	82.797
C4 *	-0.0991	0.0042	-23.648	559.231
C5 *	-0.0260	0.0043	-6.126	37.527
C6 *	0.0078	0.0042	1.846	3.408
C7 *	0.1826	0.0045	40.525	1642.294
C8 *	0.2156	0.0044	49.239	2424.493
C9 *	0.0407	0.0042	9.737	94.808
C10 *	0.0637	0.0043	14.992	224.758
C11 *	0.0000	0.0043	-0.006	0.000
C12 *	-0.0356	0.0045	-7.900	62.406
C13 *	-0.0877	0.0044	-20.040	401.613
C14 *	-0.0706	0.0042	-16.837	283.483
C15 *	-0.0163	0.0043	-3.837	14.724
C16 *	0.0080	0.0043	1.877	3.523
C17 *	0.2252	0.0045	50.304	2530.517
C18 *	0.2404	0.0044	54.758	2998.433
C19 *	0.0277	0.0043	6.496	42.199
C20 *	0.0142	0.0042	3.389	11.486
ZN1	-0.5026	0.0019	-264.406	69910.375
N5'	-2.6674	0.0036	-735.638	541162.750
				==========
SUM((D/S)**2) FOR STARRED ATOMS				16817.561

CHI-SQUARED AT 95% FOR 21 DEGREES OF FREEDOM: 32.70
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 2

M1 = -0.72647(0.00025)
M2 = -0.58804(0.00029)
M3 = -0.35560(0.00035)
D = -6.80515(0.00257)

ATOM	D	S	D/S	(D/S)**2
N1' *	0.1957	0.0035	55.394	3068.476
N2' *	0.0917	0.0035	25.954	673.592
N3' *	0.0508	0.0036	14.240	202.779
N4' *	0.1129	0.0035	31.957	1021.276

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C1' *	0.0668	0.0042	15.854	251.340
C2' *	-0.0591	0.0044	-13.505	182.387
C3' *	-0.0401	0.0044	-9.099	82.797
C4' *	0.0991	0.0042	23.648	559.231
C5' *	0.0260	0.0043	6.126	37.528
C6' *	-0.0078	0.0042	-1.846	3.408
C7' *	-0.1826	0.0045	-40.525	1642.299
C8' *	-0.2156	0.0044	-49.239	2424.478
C9' *	-0.0407	0.0042	-9.737	94.807
C10'*	-0.0637	0.0043	-14.992	224.759
C11'*	0.0000	0.0043	0.006	0.000
C12'*	0.0356	0.0045	7.900	62.405
C13'*	0.0877	0.0044	20.040	401.612
C14'*	0.0706	0.0042	16.837	283.485
C15'*	0.0163	0.0043	3.837	14.724
C16'*	-0.0080	0.0043	-1.877	3.523
C17'*	-0.2252	0.0045	-50.304	2530.518
C18'*	-0.2404	0.0044	-54.758	2998.432
C19'*	-0.0277	0.0043	-6.496	42.197
C20'*	-0.0142	0.0042	-3.389	11.487
ZN1'	0.5026	0.0019	264.406	69910.438
N5	2.6674	0.0036	735.638	541162.625
				==========
SUM((D/S)**2) FOR STARRED ATOMS				16817.537

CHI-SQUARED AT 95% FOR 21 DEGREES OF FREEDOM: 32.70
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 3

M1 = -0.74726(0.00085)
M2 = -0.55916(0.00102)
M3 = -0.35909(0.00111)
D = -3.56204(0.00285)

ATOM	D	S	D/S	(D/S)**2
N1 *	-0.0104	0.0036	-2.939	8.638
N2 *	0.0105	0.0036	2.946	8.680
N3 *	-0.0107	0.0036	-2.969	8.815
N4 *	0.0104	0.0036	2.933	8.603
ZN1	-0.3892	0.0019	-203.144	41267.328
N5'	-2.5653	0.0036	-703.376	494738.188
N4'	-2.9290	0.0036	-824.249	679385.875
N3'	-2.9079	0.0036	-810.401	656749.500
N2'	-2.9290	0.0036	-824.262	679407.813
N1'	-2.9081	0.0036	-818.377	669740.125
				==========
SUM((D/S)**2) FOR STARRED ATOMS				34.736

CHI-SQUARED AT 95% FOR 1 DEGREES OF FREEDOM: 3.84
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 4

M1 = -0.74726(0.00074)
M2 = -0.55916(0.00101)
M3 = -0.35909(0.00114)
D = -6.48059(0.00898)

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ATOM	D	S	D/S	(D/S)**2
N1' *	0.0104	0.0036	2.939	8.638
N2' *	-0.0105	0.0036	-2.946	8.681
N3' *	0.0107	0.0036	2.969	8.815
N4' *	-0.0104	0.0036	-2.933	8.603
ZN1'	0.3892	0.0019	203.144	41267.398
N5	2.5653	0.0036	703.376	494738.188
N4	2.9290	0.0036	824.249	679385.938
N3	2.9079	0.0036	810.401	656749.688
N2	2.9290	0.0036	824.262	679407.250
N1	2.9081	0.0036	818.376	669739.938
				==========
SUM((D/S)**2) FOR STARRED ATOMS				34.738

CHI-SQUARED AT 95% FOR 1 DEGREES OF FREEDOM: 3.84
THE GROUP OF ATOMS DEVIATES SIGNIFICANTLY FROM PLANARITY

PLANE 5

M1 = 0.52148(0.00136)
M2 = -0.46906(0.00159)
M3 = -0.71277(0.00120)
D = -1.86487(0.01171)

ATOM	D	S	D/S	(D/S)**2
N5' *	0.0010	0.0032	0.315	0.099
C39'*	0.0029	0.0038	0.764	0.583
C40'*	-0.0034	0.0045	-0.754	0.569
C41'*	-0.0028	0.0045	-0.630	0.397
C42'*	0.0070	0.0040	1.752	3.068
C43'*	-0.0069	0.0040	-1.709	2.922
ZN1	0.1255	0.0015	83.602	6989.302
N1	-1.3109	0.0031	-416.448	173429.016
N2	-1.1947	0.0031	-379.533	144045.031
N3	1.6680	0.0032	525.541	276193.344
N4	1.5640	0.0031	496.859	246869.141
				==========
SUM((D/S)**2) FOR STARRED ATOMS				7.639

CHI-SQUARED AT 95% FOR 3 DEGREES OF FREEDOM: 7.81
THE GROUP OF ATOMS DOES NOT DEVIATE SIGNIFICANTLY FROM PLANARITY

PLANE 6

M1 = 0.52148(0.00139)
M2 = -0.46906(0.00152)
M3 = -0.71277(0.00128)
D = -1.76434(0.01403)

ATOM	D	S	D/S	(D/S)**2
N5 *	-0.0010	0.0032	-0.315	0.099
C39 *	-0.0029	0.0038	-0.764	0.583
C40 *	0.0034	0.0045	0.754	0.569
C41 *	0.0028	0.0045	0.630	0.397
C42 *	-0.0070	0.0040	-1.752	3.068
C43 *	0.0069	0.0040	1.709	2.922
ZN1	0.0249	0.0015	16.614	276.012
N1	-1.4114	0.0031	-448.386	201050.328
N2	-1.2952	0.0031	-411.471	169308.359

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N3	1.5675	0.0032	493.866	243903.625
N4	1.4634	0.0031	464.921	216151.563
				==========
SUM((D/S)**2) FOR STARRED ATOMS				7.639

CHI-SQUARED AT 95% FOR 3 DEGREES OF FREEDOM: 7.81
THE GROUP OF ATOMS DOES NOT DEVIATE SIGNIFICANTLY FROM PLANARITY

WEIGHTED LEAST-SQUARES LINES THROUGH THE STARRED ATOMS
(SCHOEMAKER,WASER,MARSH & BERGMAN,ACTA CRYST.(1959)12,600
M1,M2,M3 ARE THE DIRECTION COSINES REFERRED TO THE X,Y,Z ORTHOGONAL AXES
X0,Y0,Z0 ARE THE COORDINATES OF THE CENTROID OF THE SET OF ATOMS
EQUATION OF THE LINE:' (X-X0)/M1=(Y-Y0)/M2=(Z-Z0)/M3

LINE 1

M1 =	-0.80971(0.00103)	X0 =	2.78169(0.00324)
M2 =	-0.45145(0.00156)	Y0 =	4.09545(0.00261)
M3 =	-0.37492(0.00127)	Z0 =	1.86766(0.00194)

ATOM	D	S	D/S	(D/S)**2
N5' *	0.0000	0.0045	0.000	0.000
ZN1 *	0.0000	0.0021	0.000	0.000
N1	1.9681	0.0044	447.932	200643.063
N2	2.0525	0.0044	467.123	218203.516
N3	2.1057	0.0045	472.546	223299.719
N4	2.0057	0.0044	456.489	208382.641
ZN1'	5.7466	0.0021	2729.584	7450631.500
N5	5.7466	0.0045	1281.164	1641382.250
C39'	1.0386	0.0053	194.467	37817.387
C40'	0.8464	0.0062	136.786	18710.475
C41'	0.4616	0.0062	74.216	5508.044
C42'	1.4995	0.0056	267.205	71398.664
C43'	1.2375	0.0056	221.838	49212.184
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

LINE 2

M1 =	0.80971(0.00099)	X0 =	1.39416(0.00324)
M2 =	0.45145(0.00151)	Y0 =	8.28423(0.00261)
M3 =	0.37492(0.00131)	Z0 =	-1.86766(0.00194)

ATOM	D	S	D/S	(D/S)**2
N5 *	0.0000	0.0045	0.000	0.000
ZN1'*	0.0000	0.0021	0.000	0.000
N1	4.6612	0.0044	1060.850	1125401.875
N2	7.4108	0.0044	1686.638	2844748.250
N3	7.3603	0.0045	1651.763	2728319.500
N4	4.5706	0.0044	1040.216	1082049.750
ZN1	5.7466	0.0021	2729.585	7450635.500
N5'	5.7466	0.0045	1281.165	1641382.875
C39	1.0386	0.0053	194.467	37817.359
C40	0.8464	0.0062	136.786	18710.422
C41	0.4616	0.0062	74.216	5508.058
C42	1.4995	0.0056	267.205	71398.766
C43	1.2375	0.0056	221.838	49212.254
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

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LINE 3

M1 =	0.85245(0.00101)	X0 =	4.85625(0.00485)
M2 =	0.29977(0.00184)	Y0 =	5.00781(0.00387)
M3 =	0.42834(0.00165)	Z0 =	2.87506(0.00330)

ATOM	D	S	D/S	(D/S)**2
N5' *	0.0000	0.0045	0.001	0.000
C41'*	0.0000	0.0062	0.001	0.000
ZN1	0.3637	0.0021	173.807	30209.002
N1	1.5584	0.0044	356.761	127278.094
N2	2.2823	0.0044	522.479	272984.188
N3	2.4284	0.0044	547.099	299316.969
N4	1.8543	0.0044	424.483	180186.188
ZN1'	5.5760	0.0021	2664.770	7101000.500
N5	5.2339	0.0045	1172.972	1375864.000
C39'	1.1589	0.0053	218.091	47563.492
C40'	1.1752	0.0061	191.361	36619.121
C42'	1.1833	0.0056	211.827	44870.617
C43'	1.1377	0.0055	205.447	42208.379
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

LINE 4

M1 =	0.44987(0.00210)	X0 =	4.85390(0.00480)
M2 =	-0.56011(0.00168)	Y0 =	4.99295(0.00399)
M3 =	0.69563(0.00140)	Z0 =	2.87487(0.00330)

ATOM	D	S	D/S	(D/S)**2
C39'*	0.0000	0.0058	0.000	0.000
C42'*	0.0000	0.0061	0.000	0.000
ZN1	3.2167	0.0025	1300.352	1690914.500
N1	3.6287	0.0048	760.535	578413.625
N2	4.3484	0.0048	911.384	830620.875
N3	4.1315	0.0048	856.346	733328.375
N4	3.4035	0.0048	713.335	508846.250
ZN1'	0.3712	0.0025	150.047	22513.965
N5	1.6645	0.0049	340.588	116000.031
N5'	1.1825	0.0049	241.964	58546.500
C40'	1.1921	0.0067	178.627	31907.529
C41'	1.2063	0.0067	178.896	32003.658
C43'	1.1439	0.0061	188.354	35477.379
				==========
SUM((D/S)**2) FOR STARRED ATOMS				0.000

DIHEDRAL ANGLES FORMED BY LSQ-PLANES

PLANE	- PLANE	ANGLE(E.S.D.)
1	2	0.00(0.03)
1	3	2.05(0.06)
1	4	2.05(0.06)
1	5	81.35(0.08)
1	6	81.35(0.09)
2	3	2.05(0.06)
2	4	2.05(0.06)
2	5	81.35(0.08)
2	6	81.35(0.08)
3	4	0.00(0.11)