Table 1. Crystal data and structure refinement for $Mg\{C(Me_2pz)_3\}\{N(SiMe_3)_2\}$ (**MGC1**)

Empirical formula	C22 H39 Mg1 N7 Si2
Formula weight	482.08
Crystal description	pale yellow block
Crystal size	0.50 x 0.25 x 0.20 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 16.3849(2) A alpha = 90 deg. b = 24.5357(4) A beta = 119.5460(10) deg. c = 16.1402(2) A gamma = 90 deg.
Reflections for cell refinement	12443
Range in theta	5 to 27 deg.
Volume, Z	5644.82(15) A^3, 8
Density (calculated)	1.134 Mg/m^3
Absorption coefficient	0.170 mm^-1
F(000)	2080
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.121 to 27.501 deg.
Index ranges	-21<=h<=18, 0<=k<=31, 0<=l<=20
Reflections collected	31644
Independent reflections	12459 [R(merge) = 0.033]
Observed reflections	7190 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.823, Tmax = 1.000)
Structure solution by	SHELXS
Hydrogen atom location	Geometric with reference to Fourier maps
Hydrogen atom treatment	Riding model
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev polynomial
Data / restraints / parameters	7190 / 0/ 577

Goodness-of-fit on F	1.1122
Final R indices [I>3sigma(I)]	R1 = 0.0427, Rw = 0.0413
Final maximum delta/sigma	0.0008
Largest diff. peak and hole	0.31 and -0.30 e.A^-3

Comments: No special comments. Two crystallographically independent molecules in the asymmetric unit. Numbering scheme for the second molecule is based on that of the first (100 added to the respective serial numbers)

Table 2. Selected bond lengths [A] and angles [deg] for **MGC1**.

Mg(1)-N(1)	2.0943(19)
Mg(1)-N(3)	2.1523(19)
Mg(1)-N(5)	2.0984(19)
Mg(1)-N(7)	1.9867(19)
N(1)-N(2)	1.383(3)
N(1)-C(1)	1.336(3)
N(2)-C(3)	1.355(3)
N(2)-C(16)	1.441(3)
N(3)-N(4)	1.399(2)
N(3)-C(6)	1.338(3)
N(4)-C(8)	1.360(3)
N(4)-C(16)	1.448(3)
N(5)-N(6)	1.380(2)
N(5)-C(11)	1.334(3)
N(6)-C(13)	1.356(3)
N(6)-C(16)	1.442(3)
N(7)-Si(1)	1.7032(19)
N(7)-Si(2)	1.6979(19)
Si(1)-C(17)	1.878(3)
Si(1)-C(18)	1.885(3)
Si(1)-C(19)	1.876(3)
Si(2)-C(20)	1.869(3)
Si(2)-C(21)	1.880(3)
Si(2)-C(22)	1.873(3)
C(1)-C(2)	1.390(4)
C(1)-C(4)	1.487(4)
C(2)-C(3)	1.370(4)
C(3)-C(5)	1.490(4)
C(6)-C(7)	1.396(3)
C(6)-C(9)	1.489(3)
C(7)-C(8)	1.369(4)
C(8)-C(10)	1.486(3)
C(11)-C(12)	1.397(3)
C(11)-C(14)	1.498(3)
C(12)-C(13)	1.369(4)
C(13)-C(15)	1.488(4)
Mg(101)-N(101)	2.1105(19)
Mg(101)-N(103)	2.1379(19)
Mg(101)-N(105)	2.077(2)
Mg(101)-N(107)	1.9878(19)
N(101)-N(102)	1.385(3)
N(101)-C(101)	1.337(3)
N(102)-C(103)	1.361(3)
N(102)-C(116)	1.445(3)
N(103)-N(104)	1.393(3)
N(103)-C(106)	1.339(3)
N(104)-C(108)	1.357(3)
N(104)-C(116)	1.452(3)
N(105)-N(106)	1.385(3)
N(105)-C(111)	1.329(3)
N(106)-C(113)	1.348(3)
N(106)-C(116)	1.446(3)
N(107)-Si(101)	1.703(2)
N(107)-Si(102)	1.6995(19)
Si(101)-C(117)	1.871(3)
Si(101)-C(118)	1.871(3)
Si(101)-C(119)	1.884(3)

Si(102)-C(120)	1.873(3)
Si(102)-C(121)	1.875(3)
Si(102)-C(122)	1.880(3)
C(101)-C(102)	1.392(3)
C(101)-C(104)	1.489(4)
C(102)-C(103)	1.370(4)
C(103)-C(105)	1.493(4)
C(106)-C(107)	1.398(4)
C(106)-C(109)	1.488(4)
C(107)-C(108)	1.365(4)
C(108)-C(110)	1.491(4)
C(111)-C(112)	1.395(4)
C(111)-C(114)	1.486(4)
C(112)-C(113)	1.372(4)
C(113)-C(115)	1.494(4)

N(1)-Mg(1)-N(3)	86.02(8)
N(1)-Mg(1)-N(5)	92.82(8)
N(3)-Mg(1)-N(5)	89.22(7)
N(1)-Mg(1)-N(7)	122.35(8)
N(3)-Mg(1)-N(7)	136.48(8)
N(5)-Mg(1)-N(7)	118.22(8)
Mg(1)-N(1)-N(2)	111.63(13)
Mg(1)-N(1)-C(1)	141.72(17)
N(2)-N(1)-C(1)	106.30(18)
N(1)-N(2)-C(3)	109.72(19)
N(1)-N(2)-C(16)	123.50(18)
C(3)-N(2)-C(16)	126.6(2)
Mg(1)-N(3)-N(4)	108.42(13)
Mg(1)-N(3)-C(6)	145.67(16)
N(4)-N(3)-C(6)	105.33(17)
N(3)-N(4)-C(8)	110.03(19)
N(3)-N(4)-C(16)	124.61(17)
C(8)-N(4)-C(16)	125.10(19)
Mg(1)-N(5)-N(6)	111.17(13)
Mg(1)-N(5)-C(11)	141.70(17)
N(6)-N(5)-C(11)	105.89(18)
N(5)-N(6)-C(13)	110.39(19)
N(5)-N(6)-C(16)	123.10(17)
C(13)-N(6)-C(16)	126.4(2)
Mg(1)-N(7)-Si(1)	119.33(10)
Mg(1)-N(7)-Si(2)	117.34(10)
Si(1)-N(7)-Si(2)	123.33(11)
N(7)-Si(1)-C(17)	113.31(14)
N(7)-Si(1)-C(18)	113.33(12)
C(17)-Si(1)-C(18)	106.66(15)
N(7)-Si(1)-C(19)	110.88(11)
C(17)-Si(1)-C(19)	105.61(14)
C(18)-Si(1)-C(19)	106.53(14)
N(7)-Si(2)-C(20)	109.49(13)
N(7)-Si(2)-C(21)	110.38(12)
C(20)-Si(2)-C(21)	109.75(16)
N(7)-Si(2)-C(22)	116.30(12)
C(20)-Si(2)-C(22)	105.38(16)
C(21)-Si(2)-C(22)	105.28(15)
N(1)-C(1)-C(2)	109.8(2)
N(1)-C(1)-C(4)	121.1(2)
C(2)-C(1)-C(4)	129.1(2)
C(1)-C(2)-C(3)	106.8(2)
C(2)-C(3)-N(2)	107.4(2)
C(2)-C(3)-C(5)	131.1(2)
N(2)-C(3)-C(5)	121.5(3)
N(3)-C(6)-C(7)	110.6(2)
N(3)-C(6)-C(9)	122.7(2)

C(7)-C(6)-C(9)	126.7(2)
C(6)-C(7)-C(8)	106.7(2)
C(7)-C(8)-N(4)	107.4(2)
C(7)-C(8)-C(10)	130.8(2)
N(4)-C(8)-C(10)	121.8(2)
N(5)-C(11)-C(12)	110.1(2)
N(5)-C(11)-C(14)	121.0(2)
C(12)-C(11)-C(14)	129.0(2)
C(11)-C(12)-C(13)	106.6(2)
C(12)-C(13)-N(6)	107.0(2)
C(12)-C(13)-C(15)	130.5(2)
N(6)-C(13)-C(15)	122.5(2)
N(4)-C(16)-N(6)	109.61(18)
N(4)-C(16)-N(2)	109.09(18)
N(6)-C(16)-N(2)	110.20(19)
N(101)-Mg(101)-N(103)	85.38(8)
N(101)-Mg(101)-N(105)	91.86(8)
N(103)-Mg(101)-N(105)	90.37(7)
N(101)-Mg(101)-N(107)	127.81(8)
N(103)-Mg(101)-N(107)	134.77(8)
N(105)-Mg(101)-N(107)	114.59(8)
Mg(101)-N(101)-N(102)	111.30(13)
Mg(101)-N(101)-C(101)	142.49(16)
N(102)-N(101)-C(101)	106.17(18)
N(101)-N(102)-C(103)	109.9(2)
N(101)-N(102)-C(116)	123.91(18)
C(103)-N(102)-C(116)	126.0(2)
Mg(101)-N(103)-N(104)	109.94(13)
Mg(101)-N(103)-C(106)	144.35(17)
N(104)-N(103)-C(106)	105.70(18)
N(103)-N(104)-C(108)	110.12(19)
N(103)-N(104)-C(116)	124.19(18)
C(108)-N(104)-C(116)	125.2(2)
Mg(101)-N(105)-N(106)	112.49(13)
Mg(101)-N(105)-C(111)	141.04(17)
N(106)-N(105)-C(111)	106.36(18)
N(105)-N(106)-C(113)	109.74(19)
N(105)-N(106)-C(116)	123.13(18)
C(113)-N(106)-C(116)	127.1(2)
Mg(101)-N(107)-Si(101)	117.26(10)
Mg(101)-N(107)-Si(102)	118.85(11)
Si(101)-N(107)-Si(102)	123.88(11)
N(107)-Si(101)-C(117)	112.48(14)
N(107)-Si(101)-C(118)	110.27(11)
C(117)-Si(101)-C(118)	109.00(16)
N(107)-Si(101)-C(119)	115.26(12)
C(117)-Si(101)-C(119)	105.49(15)
C(118)-Si(101)-C(119)	103.82(14)
N(107)-Si(102)-C(120)	109.39(12)
N(107)-Si(102)-C(121)	111.27(12)
C(120)-Si(102)-C(121)	109.54(14)
N(107)-Si(102)-C(122)	115.16(13)
C(120)-Si(102)-C(122)	105.25(17)
C(121)-Si(102)-C(122)	105.96(15)
N(101)-C(101)-C(102)	109.9(2)
N(101)-C(101)-C(104)	121.4(2)
C(102)-C(101)-C(104)	128.6(2)
C(101)-C(102)-C(103)	106.9(2)
C(102)-C(103)-N(102)	107.1(2)
C(102)-C(103)-C(105)	130.9(2)
N(102)-C(103)-C(105)	121.9(3)
N(103)-C(106)-C(107)	109.9(2)
N(103)-C(106)-C(109)	122.5(2)
C(107)-C(106)-C(109)	127.5(2)

C(106)-C(107)-C(108)	107.1(2)
C(107)-C(108)-N(104)	107.2(2)
C(107)-C(108)-C(110)	130.5(2)
N(104)-C(108)-C(110)	122.2(2)
N(105)-C(111)-C(112)	109.9(2)
N(105)-C(111)-C(114)	121.4(2)
C(112)-C(111)-C(114)	128.7(2)
C(111)-C(112)-C(113)	106.4(2)
C(112)-C(113)-N(106)	107.6(2)
C(112)-C(113)-C(115)	130.2(2)
N(106)-C(113)-C(115)	122.2(2)
N(104)-C(116)-N(106)	109.66(19)
N(104)-C(116)-N(102)	108.30(18)
N(106)-C(116)-N(102)	110.51(19)

Table 1. Crystal data and structure refinement for Mg(k2-TpmH)(N(SiMe3)2)2 (mgc2)

Empirical formula	C24 H50 Mg1 N8 Si4
Formula weight	587.36
Crystal description	white plate
Crystal size	0.20 x 0.10 x 0.10 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 11.3901(3) A alpha = 90 deg. b = 18.6622(5) A beta = 104.8343(13) deg. c = 16.4869(4) A gamma = 90 deg.
Reflections for cell refinement	7476
Range in theta	5 to 27 deg.
Volume, Z	3387.72(15) A^3, 4
Density (calculated)	1.152 Mg/m^3
Absorption coefficient	0.221 mm^-1
F(000)	1272
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.093 to 27.504 deg.
Index ranges	-14<=h<=14, 0<=k<=24, 0<=l<=21
Reflections collected	14527
Independent reflections	7686 [R(merge) = 0.054]
Observed reflections	3825 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.98, Tmax = 0.98)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Mixed - see comments
Hydrogen atom treatment	Mixed - see comments
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev
Data / restraints / parameters	3825 / 0/ 350

Goodness-of-fit on F	1.1400
Final R indices [I>3sigma(I)]	R1 = 0.0464, Rw = 0.0457
Final maximum delta/sigma	0.0004
Largest diff. peak and hole	0.44 and -0.41 e.A^-3

Comments:
H atoms bound to Si were located from Fourier maps and positionally refined in an isotropic approximation. C-bound H atoms were placed in calculated positions and refined in a riding model

Table 2. Selected bond lengths [A] and angles [deg] for mgc2.

Mg(1)-N(1)	2.147(3)
Mg(1)-N(3)	2.139(3)
Mg(1)-N(7)	2.008(3)
Mg(1)-N(8)	2.024(3)
N(1)-N(2)	1.380(3)
N(1)-C(1)	1.339(4)
N(2)-C(3)	1.368(4)
N(2)-C(16)	1.432(4)
N(3)-N(4)	1.375(3)
N(3)-C(6)	1.330(4)
N(4)-C(8)	1.361(4)
N(4)-C(16)	1.445(4)
N(5)-N(6)	1.380(3)
N(5)-C(11)	1.325(4)
N(6)-C(13)	1.375(4)
N(6)-C(16)	1.463(4)
N(7)-Si(1)	1.698(3)
N(7)-Si(2)	1.694(3)
N(8)-Si(3)	1.697(3)
N(8)-Si(4)	1.702(3)
Si(1)-C(17)	1.857(4)
Si(1)-C(18)	1.871(4)
Si(2)-C(19)	1.865(4)
Si(2)-C(20)	1.854(4)
Si(3)-C(21)	1.857(4)
Si(3)-C(22)	1.848(4)
Si(4)-C(23)	1.864(4)
Si(4)-C(24)	1.861(4)
C(1)-C(2)	1.408(4)
C(1)-C(4)	1.495(4)
C(2)-C(3)	1.361(5)
C(3)-C(5)	1.501(4)
C(6)-C(7)	1.410(4)
C(6)-C(9)	1.493(4)
C(7)-C(8)	1.364(4)
C(8)-C(10)	1.499(4)
C(11)-C(12)	1.410(5)
C(11)-C(14)	1.493(5)
C(12)-C(13)	1.363(5)
C(13)-C(15)	1.491(4)
N(1)-Mg(1)-N(3)	87.06(10)
N(1)-Mg(1)-N(7)	112.62(11)
N(3)-Mg(1)-N(7)	111.35(11)
N(1)-Mg(1)-N(8)	104.09(11)
N(3)-Mg(1)-N(8)	106.26(11)
N(7)-Mg(1)-N(8)	127.76(11)
Mg(1)-N(1)-N(2)	124.80(18)
Mg(1)-N(1)-C(1)	128.7(2)
N(2)-N(1)-C(1)	105.1(2)
N(1)-N(2)-C(3)	111.4(2)
N(1)-N(2)-C(16)	122.1(2)
C(3)-N(2)-C(16)	126.2(3)
Mg(1)-N(3)-N(4)	124.15(18)
Mg(1)-N(3)-C(6)	128.2(2)
N(4)-N(3)-C(6)	105.3(2)
N(3)-N(4)-C(8)	111.3(2)
N(3)-N(4)-C(16)	122.3(2)
C(8)-N(4)-C(16)	125.9(2)

N(6)-N(5)-C(11)	104.8(3)
N(5)-N(6)-C(13)	111.7(2)
N(5)-N(6)-C(16)	113.5(2)
C(13)-N(6)-C(16)	130.8(3)
Mg(1)-N(7)-Si(1)	117.14(14)
Mg(1)-N(7)-Si(2)	119.27(14)
Si(1)-N(7)-Si(2)	123.51(16)
Mg(1)-N(8)-Si(3)	124.37(15)
Mg(1)-N(8)-Si(4)	115.56(13)
Si(3)-N(8)-Si(4)	120.05(16)
N(7)-Si(1)-C(17)	115.26(16)
N(7)-Si(1)-C(18)	114.41(15)
C(17)-Si(1)-C(18)	107.47(19)
N(7)-Si(2)-C(19)	114.19(17)
N(7)-Si(2)-C(20)	115.48(18)
C(19)-Si(2)-C(20)	106.2(2)
N(8)-Si(3)-C(21)	112.32(15)
N(8)-Si(3)-C(22)	115.13(17)
C(21)-Si(3)-C(22)	107.1(2)
N(8)-Si(4)-C(23)	114.24(16)
N(8)-Si(4)-C(24)	115.13(17)
C(23)-Si(4)-C(24)	105.21(19)
N(1)-C(1)-C(2)	110.2(3)
N(1)-C(1)-C(4)	121.2(3)
C(2)-C(1)-C(4)	128.6(3)
C(1)-C(2)-C(3)	107.1(3)
N(2)-C(3)-C(2)	106.2(3)
N(2)-C(3)-C(5)	122.7(3)
C(2)-C(3)-C(5)	131.1(3)
N(3)-C(6)-C(7)	110.4(3)
N(3)-C(6)-C(9)	122.5(3)
C(7)-C(6)-C(9)	127.0(3)
C(6)-C(7)-C(8)	106.4(3)
C(7)-C(8)-N(4)	106.6(3)
C(7)-C(8)-C(10)	129.9(3)
N(4)-C(8)-C(10)	123.5(3)
N(5)-C(11)-C(12)	110.9(3)
N(5)-C(11)-C(14)	121.7(3)
C(12)-C(11)-C(14)	127.4(3)
C(11)-C(12)-C(13)	106.9(3)
N(6)-C(13)-C(12)	105.6(3)
N(6)-C(13)-C(15)	127.3(3)
C(12)-C(13)-C(15)	127.1(3)
N(6)-C(16)-N(4)	110.5(2)
N(6)-C(16)-N(2)	111.9(2)
N(4)-C(16)-N(2)	113.7(2)

Table 1. Crystal data and structure refinement for Ca{C(Me2pz)3}{N(SiMe3)2}(THF) (adscw25)

Empirical formula	C26 H47 Ca N7 O Si2
Formula weight	569.96
Crystal description	white block
Crystal size	0.30 x 0.15 x 0.15 mm
Temperature	150 K
Crystal system	Monoclinic

Space group	C 2/c
Unit cell dimensions	a = 39.3059(4) A alpha = 90 deg. b = 8.5990(16) A beta = 110.691(2) deg. c = 20.6529(8) A gamma = 90 deg.
Reflections for cell refinement	12535
Range in theta	5 to 28 deg.
Volume, Z	6530.3(12) A^3, 8
Density (calculated)	1.159 Mg/m^3
Absorption coefficient	0.295 mm^-1
F(000)	2464
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Index ranges	-50<=h<=46, 0<=k<=11, 0<=l<=26
Reflections collected	24497
Theta range for data collection	5.149 to 27.243 deg.
Independent reflections	7216 [R(merge) = 0.101]
Reflections with I>2sigma(I)	2899
Absorption correction	Semi-empirical from equivalents (Tmin = 0.96, Tmax = 0.96)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Geometric
Hydrogen atom treatment	Riding
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	Auto-statistical
Data / restraints / parameters	7216 / 0/ 343
Goodness-of-fit on F^2	0.9778
R1 [I>2sigma(I)] =	0.0981
wR2 (all data) =	0.3168
Final maximum delta/sigma	0.0004
Largest diff. peak and hole	1.05 and -0.95 e.A^-3

Comments: The crystal was a very weak diffractor with an average I/sigma(I) of only 3.5. Nonetheless structure solution and subsequent refinement were straightforward and satisfactorily

converged to a model which is more than adequate to establish confidently the overall connectivity. One of the carbon atoms of the THF ligand was found to be disordered over two sites (C(25) and C(251))

Table 2. Selected bond lengths [A] and angles [deg] for adscw25.

Ca(1)-N(1)	2.436(7)
Ca(1)-N(3)	2.412(6)
Ca(1)-N(5)	2.454(6)
Ca(1)-N(7)	2.322(6)
Ca(1)-O(1)	2.398(6)
N(1)-N(2)	1.394(8)
N(1)-C(1)	1.338(10)
N(2)-C(3)	1.350(10)
N(2)-C(16)	1.465(10)
N(3)-N(4)	1.386(9)
N(3)-C(6)	1.340(10)
N(4)-C(8)	1.350(10)
N(4)-C(16)	1.458(10)
N(5)-N(6)	1.398(8)
N(5)-C(11)	1.351(10)
N(6)-C(13)	1.345(10)
N(6)-C(16)	1.418(11)
N(7)-Si(1)	1.690(7)
N(7)-Si(2)	1.690(7)
O(1)-C(23)	1.451(10)
O(1)-C(26)	1.435(10)
Si(1)-C(17)	1.865(9)
Si(1)-C(18)	1.884(9)
Si(1)-C(19)	1.891(9)
Si(2)-C(20)	1.857(9)
Si(2)-C(21)	1.881(10)
Si(2)-C(22)	1.870(9)
C(1)-C(2)	1.439(11)
C(1)-C(4)	1.469(11)
C(2)-C(3)	1.350(11)
C(3)-C(5)	1.480(11)
C(15)-C(13)	1.531(11)
C(6)-C(7)	1.395(11)
C(6)-C(9)	1.501(12)
C(7)-C(8)	1.371(12)
C(8)-C(10)	1.491(11)
C(11)-C(12)	1.355(11)
C(11)-C(14)	1.513(12)
C(12)-C(13)	1.363(12)
C(23)-C(24)	1.514(14)
C(24)-C(25)	1.50(3)
C(24)-C(251)	1.48(3)
C(26)-C(25)	1.44(3)
C(26)-C(251)	1.46(3)
N(1)-Ca(1)-N(3)	78.8(2)
N(1)-Ca(1)-N(5)	77.3(2)
N(3)-Ca(1)-N(5)	78.7(2)
N(1)-Ca(1)-N(7)	104.1(2)
N(3)-Ca(1)-N(7)	125.3(2)
N(5)-Ca(1)-N(7)	155.9(2)
N(1)-Ca(1)-O(1)	158.4(2)
N(3)-Ca(1)-O(1)	84.7(2)
N(5)-Ca(1)-O(1)	85.9(2)
N(7)-Ca(1)-O(1)	96.8(2)
Ca(1)-N(1)-N(2)	116.4(5)
Ca(1)-N(1)-C(1)	136.7(5)
N(2)-N(1)-C(1)	106.3(6)
N(1)-N(2)-C(3)	110.4(6)
N(1)-N(2)-C(16)	123.8(6)

C(3)-N(2)-C(16)	125.8(7)
Ca(1)-N(3)-N(4)	117.5(5)
Ca(1)-N(3)-C(6)	137.0(5)
N(4)-N(3)-C(6)	105.0(6)
N(3)-N(4)-C(8)	110.8(7)
N(3)-N(4)-C(16)	123.2(6)
C(8)-N(4)-C(16)	125.9(7)
Ca(1)-N(5)-N(6)	115.4(5)
Ca(1)-N(5)-C(11)	139.0(5)
N(6)-N(5)-C(11)	104.2(6)
N(5)-N(6)-C(13)	109.4(7)
N(5)-N(6)-C(16)	124.8(6)
C(13)-N(6)-C(16)	125.8(7)
Ca(1)-N(7)-Si(1)	119.3(3)
Ca(1)-N(7)-Si(2)	114.1(3)
Si(1)-N(7)-Si(2)	126.6(4)
Ca(1)-O(1)-C(23)	125.9(5)
Ca(1)-O(1)-C(26)	124.5(5)
C(23)-O(1)-C(26)	109.0(6)
N(7)-Si(1)-C(17)	113.3(4)
N(7)-Si(1)-C(18)	115.3(4)
C(17)-Si(1)-C(18)	105.8(5)
N(7)-Si(1)-C(19)	110.2(4)
C(17)-Si(1)-C(19)	106.6(5)
C(18)-Si(1)-C(19)	104.9(5)
N(7)-Si(2)-C(20)	116.1(4)
N(7)-Si(2)-C(21)	106.8(4)
C(20)-Si(2)-C(21)	106.4(5)
N(7)-Si(2)-C(22)	114.1(4)
C(20)-Si(2)-C(22)	105.8(5)
C(21)-Si(2)-C(22)	107.0(5)
N(1)-C(1)-C(2)	108.4(7)
N(1)-C(1)-C(4)	123.6(7)
C(2)-C(1)-C(4)	127.9(8)
C(1)-C(2)-C(3)	106.9(7)
N(2)-C(3)-C(2)	108.0(7)
N(2)-C(3)-C(5)	123.0(8)
C(2)-C(3)-C(5)	129.0(8)
N(3)-C(6)-C(7)	110.7(7)
N(3)-C(6)-C(9)	121.9(7)
C(7)-C(6)-C(9)	127.3(8)
C(6)-C(7)-C(8)	106.2(7)
C(7)-C(8)-N(4)	107.4(7)
C(7)-C(8)-C(10)	131.0(8)
N(4)-C(8)-C(10)	121.6(8)
N(5)-C(11)-C(12)	111.7(8)
N(5)-C(11)-C(14)	120.3(7)
C(12)-C(11)-C(14)	127.9(8)
C(11)-C(12)-C(13)	106.3(8)
C(15)-C(13)-C(12)	130.4(8)
C(15)-C(13)-N(6)	121.2(8)
C(12)-C(13)-N(6)	108.4(7)
N(2)-C(16)-N(4)	110.3(6)
N(2)-C(16)-N(6)	110.8(6)
N(4)-C(16)-N(6)	112.3(7)
O(1)-C(23)-C(24)	106.3(7)
C(23)-C(24)-C(25)	103.6(14)
C(23)-C(24)-C(251)	105.0(14)
C(25)-C(24)-C(251)	30.5(11)
O(1)-C(26)-C(25)	107.8(14)
O(1)-C(26)-C(251)	106.7(14)
C(25)-C(26)-C(251)	31.3(12)
C(24)-C(25)-C(26)	106.0(17)
C(24)-C(251)-C(26)	105.8(18)

Table 1. Crystal data and structure refinement for adscw35.

Empirical formula	C32 H42 Ca N12 · 2(C_6H_6)
Formula weight	791.07
Crystal description	white plate
Crystal size	0.50 x 0.40 x 0.30 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 8.4830(2) A alpha = 90 deg. b = 10.2774(3) A beta = 93.2483(11) deg. c = 24.3896(9) A gamma = 90 deg.
Reflections for cell refinement	2439
Range in theta	5 to 27 deg.
Volume, Z	2122.95(11) A^3, 2
Density (calculated)	1.237 Mg/m^3
Absorption coefficient	0.195 mm^-1
F(000)	844
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.110 to 27.408 deg.
Index ranges	-10<=h<=10, 0<=k<=13, 0<=l<=31
Reflections collected	6654
Independent reflections	4332 [R(merge) = 0.042]
Observed reflections	3233 [I>3sigma(I)]
Absorption correction	Multi-scan (Tmin = 0.93, Tmax = 0.94)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Geomtric and Fourier
Hydrogen atom treatment	Riding
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev
Data / restraints / parameters	3233 / 0/ 259
Goodness-of-fit on F	1.0588

Final R indices [I>3sigma(I)]	R1 = 0.0583, Rw = 0.0632
Final maximum delta/sigma	0.0003
Largest diff. peak and hole	0.26 and -0.35 e.A^-3

Comments: No special details

Table 2. Selected bond lengths [A] and angles [deg] for adscw35.

Ca(1)-N(3A)	2.459(2)
Ca(1)-N(5A)	2.448(2)
Ca(1)-N(1A)	2.437(2)
Ca(1)-N(1)	2.437(2)
Ca(1)-N(3)	2.459(2)
Ca(1)-N(5)	2.448(2)
N(1)-N(2)	1.383(2)
N(1)-C(1)	1.345(3)
N(2)-C(3)	1.352(3)
N(2)-C(16)	1.448(2)
N(3)-N(4)	1.383(2)
N(3)-C(6)	1.334(3)
N(4)-C(8)	1.361(2)
N(4)-C(16)	1.443(3)
N(5)-N(6)	1.383(2)
N(5)-C(11)	1.330(3)
N(6)-C(13)	1.358(3)
N(6)-C(16)	1.449(2)
C(1)-C(2)	1.390(3)
C(1)-C(4)	1.496(3)
C(2)-C(3)	1.366(3)
C(3)-C(5)	1.496(3)
C(6)-C(7)	1.404(3)
C(6)-C(9)	1.495(3)
C(7)-C(8)	1.381(3)
C(8)-C(10)	1.486(3)
C(11)-C(12)	1.401(3)
C(11)-C(14)	1.495(3)
C(12)-C(13)	1.374(3)
C(13)-C(15)	1.491(3)
C(101)-C(102)	1.380(4)
C(101)-C(106)	1.391(4)
C(102)-C(103)	1.372(4)
C(103)-C(104)	1.378(4)
C(104)-C(105)	1.378(4)
C(105)-C(106)	1.378(4)

N(3A) -Ca(1)-N(5A)	75.48(6)
N(3A) -Ca(1)-N(1A)	77.81(6)
N(5A) -Ca(1)-N(1A)	77.43(6)
N(3A) -Ca(1)-N(1)	102.19(6)
N(5A) -Ca(1)-N(1)	102.57(6)
N(1A) -Ca(1)-N(1)	179.995
N(3A) -Ca(1)-N(3)	179.995
N(5A) -Ca(1)-N(3)	104.52(6)
N(1A) -Ca(1)-N(3)	102.19(6)
N(1)-Ca(1)-N(3)	77.81(6)
N(3A) -Ca(1)-N(5)	104.52(6)
N(5A) -Ca(1)-N(5)	179.995
N(1A) -Ca(1)-N(5)	102.57(6)
N(1)-Ca(1)-N(5)	77.43(6)
N(3)-Ca(1)-N(5)	75.48(6)
Ca(1)-N(1)-N(2)	118.24(12)
Ca(1)-N(1)-C(1)	136.3(2)
N(2)-N(1)-C(1)	105.3(2)
N(1)-N(2)-C(3)	110.5(2)
N(1)-N(2)-C(16)	124.3(2)
C(3)-N(2)-C(16)	125.2(2)
Ca(1)-N(3)-N(4)	117.36(11)
Ca(1)-N(3)-C(6)	136.04(14)

N(4)-N(3)-C(6)	106.4(2)
N(3)-N(4)-C(8)	110.0(2)
N(3)-N(4)-C(16)	124.7(2)
C(8)-N(4)-C(16)	125.3(2)
Ca(1)-N(5)-N(6)	118.00(11)
Ca(1)-N(5)-C(11)	136.4(2)
N(6)-N(5)-C(11)	105.5(2)
N(5)-N(6)-C(13)	110.5(2)
N(5)-N(6)-C(16)	124.3(2)
C(13)-N(6)-C(16)	125.1(2)
N(1)-C(1)-C(2)	110.2(2)
N(1)-C(1)-C(4)	119.9(2)
C(2)-C(1)-C(4)	129.9(2)
C(1)-C(2)-C(3)	106.7(2)
C(2)-C(3)-N(2)	107.3(2)
C(2)-C(3)-C(5)	131.0(2)
N(2)-C(3)-C(5)	121.7(2)
N(3)-C(6)-C(7)	110.3(2)
N(3)-C(6)-C(9)	120.6(2)
C(7)-C(6)-C(9)	129.1(2)
C(6)-C(7)-C(8)	105.9(2)
C(7)-C(8)-N(4)	107.5(2)
C(7)-C(8)-C(10)	130.7(2)
N(4)-C(8)-C(10)	121.9(2)
N(5)-C(11)-C(12)	110.8(2)
N(5)-C(11)-C(14)	120.5(2)
C(12)-C(11)-C(14)	128.7(2)
C(11)-C(12)-C(13)	106.0(2)
C(12)-C(13)-N(6)	107.2(2)
C(12)-C(13)-C(15)	130.5(2)
N(6)-C(13)-C(15)	122.3(2)
N(6)-C(16)-N(2)	110.4(2)
N(6)-C(16)-N(4)	110.6(2)
N(2)-C(16)-N(4)	110.8(2)
C(102)-C(101)-C(106)	119.5(2)
C(101)-C(102)-C(103)	120.4(2)
C(102)-C(103)-C(104)	120.3(2)
C(103)-C(104)-C(105)	119.7(2)
C(104)-C(105)-C(106)	120.5(2)
C(101)-C(106)-C(105)	119.6(2)

Symmetry transformations used to generate equivalent atoms
Carrying the suffix ‘A’: -x,1-y,1-z

Table 1. Crystal data and structure refinement for $Zn\{C(Me_2pz)_3\}Cl$ (mgc17)

Empirical formula	C16 H21 Cl1 N6 Zn1
Formula weight	398.22
Crystal description	none block
Crystal size	0.10 x 0.10 x 0.10 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 2_1
Unit cell dimensions	a = 7.8808(3) A alpha = 90 deg. b = 17.5757(6) A beta = 90.2820(15) deg. c = 13.2885(5) A gamma = 90 deg.
Reflections for cell refinement	4221
Range in theta	5 to 27 deg.
Volume, Z	1840.58(12) A^3, 4
Density (calculated)	1.437 Mg/m^3
Absorption coefficient	1.489 mm^-1
F(000)	824
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.155 to 27.439 deg.
Index ranges	-10<=h<=10, -22<=k<=22, 0<=l<=17
Reflections collected	8176
Independent reflections	8165 [R(merge) = 0.000]
Observed reflections	6609 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.86, Tmax = 0.86)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Geometric
Hydrogen atom treatment	Riding model
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev polynomial
Data / restraints / parameters	6609 / 1/ 435

Goodness-of-fit on F	1.0785
Final R indices [I>3sigma(I)]	R1 = 0.0703, Rw = 0.0721
Absolute structure parameter	Could not be detrmined
Final maximum delta/sigma	0.0002
Largest diff. peak and hole	1.75 and -1.68 e.A^-3

Comments:
Crystals of Zn(Tpmd)Cl were twinned. The twinning was satisfactorily resolved and refinement proceeded normally. H atoms were placed in calculation positions, the orientations of the methyl groups having been confirmed by reference to a Fourier difference map. Because of the twinning a satisfactory refinement of the Flack parameter could not be carried out.

Table 2. Bond lengths [A] and angles [deg] for mgc17.

Zn(1)-Cl(1)	2.152(3)
Zn(1)-N(1)	1.999(6)
Zn(1)-N(3)	2.013(6)
Zn(1)-N(5)	2.016(7)
N(1)-N(2)	1.392(9)
N(1)-C(1)	1.350(9)
N(2)-C(3)	1.400(9)
N(2)-C(16)	1.435(8)
N(3)-N(4)	1.379(9)
N(3)-C(6)	1.325(9)
N(4)-C(8)	1.370(10)
N(4)-C(16)	1.442(9)
N(5)-N(6)	1.381(10)
N(5)-C(11)	1.345(8)
N(6)-C(13)	1.354(11)
N(6)-C(16)	1.444(10)
C(1)-C(2)	1.400(11)
C(1)-C(4)	1.463(11)
C(2)-C(3)	1.369(12)
C(3)-C(5)	1.501(12)
C(6)-C(7)	1.388(12)
C(6)-C(9)	1.496(12)
C(7)-C(8)	1.367(13)
C(8)-C(10)	1.480(14)
C(11)-C(12)	1.368(14)
C(11)-C(14)	1.517(15)
C(12)-C(13)	1.380(15)
C(13)-C(15)	1.472(16)
Zn(101)-Cl(101)	2.171(2)
Zn(101)-N(101)	2.008(6)
Zn(101)-N(103)	2.017(5)
Zn(101)-N(105)	2.016(5)
N(12)-N(101)	1.389(9)
N(12)-C(103)	1.387(10)
N(12)-C(116)	1.433(10)
N(101)-C(101)	1.346(9)
N(103)-N(104)	1.398(9)
N(103)-C(106)	1.354(9)
N(104)-C(108)	1.377(9)
N(104)-C(116)	1.428(10)
N(105)-N(106)	1.388(8)
N(105)-C(111)	1.331(8)
N(106)-C(113)	1.355(9)
N(106)-C(116)	1.451(9)
C(101)-C(102)	1.405(13)
C(101)-C(104)	1.491(13)
C(102)-C(103)	1.408(14)
C(103)-C(105)	1.467(14)
C(106)-C(107)	1.393(11)
C(106)-C(109)	1.484(13)
C(107)-C(108)	1.365(13)
C(108)-C(110)	1.471(12)
C(111)-C(112)	1.405(10)
C(111)-C(114)	1.478(11)
C(112)-C(113)	1.399(10)
C(113)-C(115)	1.470(11)
Cl(1)-Zn(1)-N(1)	124.6(2)

Cl(1)-Zn(1)-N(3)	124.9(2)
N(1)-Zn(1)-N(3)	92.1(2)
Cl(1)-Zn(1)-N(5)	122.9(2)
N(1)-Zn(1)-N(5)	91.6(2)
N(3)-Zn(1)-N(5)	91.1(3)
Zn(1)-N(1)-N(2)	110.7(4)
Zn(1)-N(1)-C(1)	142.6(5)
N(2)-N(1)-C(1)	106.7(6)
N(1)-N(2)-C(3)	108.1(6)
N(1)-N(2)-C(16)	123.3(6)
C(3)-N(2)-C(16)	128.6(6)
Zn(1)-N(3)-N(4)	111.2(4)
Zn(1)-N(3)-C(6)	141.6(6)
N(4)-N(3)-C(6)	107.0(7)
N(3)-N(4)-C(8)	109.3(7)
N(3)-N(4)-C(16)	122.7(6)
C(8)-N(4)-C(16)	128.0(7)
Zn(1)-N(5)-N(6)	112.0(4)
Zn(1)-N(5)-C(11)	142.0(6)
N(6)-N(5)-C(11)	106.0(7)
N(5)-N(6)-C(13)	109.6(8)
N(5)-N(6)-C(16)	121.6(6)
C(13)-N(6)-C(16)	128.8(8)
N(1)-C(1)-C(2)	110.6(7)
N(1)-C(1)-C(4)	120.7(7)
C(2)-C(1)-C(4)	128.6(7)
C(1)-C(2)-C(3)	106.3(6)
N(2)-C(3)-C(2)	108.3(7)
N(2)-C(3)-C(5)	119.8(7)
C(2)-C(3)-C(5)	131.9(7)
N(3)-C(6)-C(7)	109.7(8)
N(3)-C(6)-C(9)	120.4(8)
C(7)-C(6)-C(9)	129.6(7)
C(6)-C(7)-C(8)	107.2(7)
N(4)-C(8)-C(7)	106.7(7)
N(4)-C(8)-C(10)	121.6(9)
C(7)-C(8)-C(10)	131.7(8)
N(5)-C(11)-C(12)	110.3(8)
N(5)-C(11)-C(14)	118.8(8)
C(12)-C(11)-C(14)	130.9(8)
C(11)-C(12)-C(13)	106.8(7)
C(12)-C(13)-N(6)	107.3(9)
C(12)-C(13)-C(15)	129.7(9)
N(6)-C(13)-C(15)	123.0(10)
N(6)-C(16)-N(4)	107.7(6)
N(6)-C(16)-N(2)	110.5(6)
N(4)-C(16)-N(2)	109.5(6)

Cl(101)-Zn(101)-N(101)	123.5(2)
Cl(101)-Zn(101)-N(103)	122.96(19)
N(101)-Zn(101)-N(103)	92.3(2)
Cl(101)-Zn(101)-N(105)	124.04(17)
N(101)-Zn(101)-N(105)	92.6(2)
N(103)-Zn(101)-N(105)	92.3(2)
N(101)-N(12)-C(103)	110.1(7)
N(101)-N(12)-C(116)	123.5(6)
C(103)-N(12)-C(116)	126.3(7)
N(12)-N(101)-Zn(101)	110.0(4)
N(12)-N(101)-C(101)	107.1(6)
Zn(101)-N(101)-C(101)	142.6(6)
Zn(101)-N(103)-N(104)	109.5(4)
Zn(101)-N(103)-C(106)	142.9(6)
N(104)-N(103)-C(106)	107.5(6)

N(103)-N(104)-C(108)	108.7(6)
N(103)-N(104)-C(116)	123.6(6)
C(108)-N(104)-C(116)	127.6(7)
Zn(101)-N(105)-N(106)	110.5(4)
Zn(101)-N(105)-C(111)	142.7(5)
N(106)-N(105)-C(111)	106.8(5)
N(105)-N(106)-C(113)	110.2(5)
N(105)-N(106)-C(116)	122.5(6)
C(113)-N(106)-C(116)	127.3(6)
N(101)-C(101)-C(102)	109.8(8)
N(101)-C(101)-C(104)	120.8(8)
C(102)-C(101)-C(104)	129.4(8)
C(101)-C(102)-C(103)	107.0(7)
C(102)-C(103)-N(12)	105.9(8)
C(102)-C(103)-C(105)	131.1(8)
N(12)-C(103)-C(105)	122.9(9)
N(103)-C(106)-C(107)	107.9(8)
N(103)-C(106)-C(109)	120.9(7)
C(107)-C(106)-C(109)	131.2(8)
C(106)-C(107)-C(108)	109.1(7)
N(104)-C(108)-C(107)	106.8(7)
N(104)-C(108)-C(110)	121.8(8)
C(107)-C(108)-C(110)	131.4(8)
N(105)-C(111)-C(112)	109.9(6)
N(105)-C(111)-C(114)	121.8(7)
C(112)-C(111)-C(114)	128.2(6)
C(111)-C(112)-C(113)	106.2(6)
C(112)-C(113)-N(106)	106.8(6)
C(112)-C(113)-C(115)	129.7(7)
N(106)-C(113)-C(115)	123.4(7)
N(106)-C(116)-N(12)	108.5(7)
N(106)-C(116)-N(104)	110.3(6)
N(12)-C(116)-N(104)	108.9(6)

```
_chemical_name_systematic
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Zn{C(Me2pz)3}{N(SiMe3)2}
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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'N'  'N'   0.0061   0.0033
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Zn'  'Zn'   0.2839   1.4301
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 '-x+1/2, y+1/2, -z+1/2'
 '-x, -y, -z'
 'x-1/2, -y-1/2, z-1/2'

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_cell_length_c                    14.299(3)
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_cell_angle_beta                  90.57(3)
_cell_angle_gamma                 90.00
_cell_volume                      2803.4(10)
_cell_formula_units_Z             4
_cell_measurement_temperature     200(2)
_cell_measurement_reflns_used     19017
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_computing_cell_refinement      'CrysAlis Red'
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_extinction_coef        ?
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N1 N 0.5992(6) 0.50614(19) 0.2721(3) 0.0518(12) Uani 1 1 d . . .
C1 C 0.4217(7) 0.5165(2) 0.2775(4) 0.0520(15) Uani 1 1 d . . .
Si2 Si 0.4363(3) 0.29070(8) 0.10655(15) 0.0803(7) Uani 1 1 d . . .
N2 N 0.6607(5) 0.45616(19) 0.2428(3) 0.0486(12) Uani 1 1 d . . .
N3 N 0.3478(5) 0.50946(18) 0.1857(3) 0.0458(12) Uani 1 1 d . . .
N4 N 0.3661(5) 0.46180(19) 0.1319(3) 0.0462(12) Uani 1 1 d . . .
N5 N 0.3465(6) 0.4793(2) 0.3418(3) 0.0562(13) Uani 1 1 d . . .
N6 N 0.3395(6) 0.4233(2) 0.3252(3) 0.0555(13) Uani 1 1 d . . .
N7 N 0.5160(6) 0.32258(19) 0.2014(4) 0.0591(14) Uani 1 1 d . . .
C10 C 0.6874(10) 0.6013(3) 0.3103(6) 0.089(2) Uani 1 1 d . . .
H10A H 0.6363 0.6203 0.2569 0.133 Uiso 1 1 calc R . .
H10B H 0.7916 0.6196 0.3274 0.133 Uiso 1 1 calc R . .
H10C H 0.6118 0.6024 0.3635 0.133 Uiso 1 1 calc R . .
C11 C 0.7218(8) 0.5423(3) 0.2844(4) 0.0586(17) Uani 1 1 d . . .
C12 C 0.8665(8) 0.5152(3) 0.2649(5) 0.0649(18) Uani 1 1 d . . .
H12 H 0.9754 0.5300 0.2686 0.078 Uiso 1 1 calc R . .
C13 C 0.8241(7) 0.4627(3) 0.2392(5) 0.0566(17) Uani 1 1 d . . .
C14 C 0.9326(8) 0.4177(3) 0.2046(6) 0.085(2) Uani 1 1 d . . .
H14A H 0.9879 0.3998 0.2578 0.127 Uiso 1 1 calc R . .
H14B H 1.0161 0.4330 0.1627 0.127 Uiso 1 1 calc R . .
H14C H 0.8651 0.3906 0.1706 0.127 Uiso 1 1 calc R . .
C20 C 0.2335(9) 0.6030(3) 0.1757(6) 0.082(2) Uani 1 1 d . . .
H20A H 0.1657 0.5991 0.2318 0.123 Uiso 1 1 calc R . .
H20B H 0.1739 0.6254 0.1293 0.123 Uiso 1 1 calc R . .
H20C H 0.3387 0.6209 0.1922 0.123 Uiso 1 1 calc R . .
C21 C 0.2670(7) 0.5481(3) 0.1359(5) 0.0563(16) Uani 1 1 d . . .
C22 C 0.2339(8) 0.5264(3) 0.0510(5) 0.0651(19) Uani 1 1 d . . .
H22 H 0.1771 0.5443 0.0010 0.078 Uiso 1 1 calc R . .
C23 C 0.2976(7) 0.4735(3) 0.0494(4) 0.0544(16) Uani 1 1 d . . .
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C24 C 0.2982(9) 0.4347(3) -0.0307(5) 0.074(2) Uani 1 1 d . . .
H24A H 0.3531 0.4005 -0.0119 0.110 Uiso 1 1 calc R . .
H24B H 0.3581 0.4513 -0.0829 0.110 Uiso 1 1 calc R . .
H24C H 0.1838 0.4269 -0.0502 0.110 Uiso 1 1 calc R . .
C30 C 0.2621(11) 0.5479(4) 0.4594(6) 0.109(3) Uani 1 1 d . . .
H30A H 0.3725 0.5588 0.4818 0.164 Uiso 1 1 calc R . .
H30B H 0.1836 0.5495 0.5112 0.164 Uiso 1 1 calc R . .
H30C H 0.2258 0.5730 0.4096 0.164 Uiso 1 1 calc R . .
C31 C 0.2688(9) 0.4909(4) 0.4223(5) 0.083(2) Uani 1 1 d . . .
C32 C 0.2070(9) 0.4430(4) 0.4566(6) 0.090(3) Uani 1 1 d . . .
H32 H 0.1440 0.4385 0.5118 0.108 Uiso 1 1 calc R . .
C33 C 0.2539(8) 0.4021(3) 0.3954(5) 0.067(2) Uani 1 1 d . . .
C34 C 0.2160(9) 0.3427(3) 0.3985(5) 0.093(3) Uani 1 1 d . . .
H34A H 0.2310 0.3267 0.3363 0.140 Uiso 1 1 calc R . .
H34B H 0.1010 0.3374 0.4181 0.140 Uiso 1 1 calc R . .
H34C H 0.2909 0.3246 0.4433 0.140 Uiso 1 1 calc R . .
C200 C 0.5520(15) 0.3086(4) -0.0003(7) 0.154(5) Uani 1 1 d . . .
H20G H 0.5485 0.3485 -0.0098 0.231 Uiso 1 1 calc R . .
H20H H 0.5012 0.2901 -0.0544 0.231 Uiso 1 1 calc R . .
H20I H 0.6675 0.2967 0.0066 0.231 Uiso 1 1 calc R . .
C201 C 0.2141(11) 0.3095(4) 0.0910(6) 0.108(3) Uani 1 1 d . . .
H20J H 0.1493 0.2934 0.1417 0.161 Uiso 1 1 calc R . .
H20K H 0.1733 0.2954 0.0308 0.161 Uiso 1 1 calc R . .
H20L H 0.2027 0.3496 0.0923 0.161 Uiso 1 1 calc R . .
C202 C 0.4463(18) 0.2121(3) 0.1144(7) 0.157(5) Uani 1 1 d . . .
H20M H 0.5569 0.2009 0.1362 0.235 Uiso 1 1 calc R . .
H20N H 0.4242 0.1962 0.0526 0.235 Uiso 1 1 calc R . .
H20O H 0.3629 0.1991 0.1586 0.235 Uiso 1 1 calc R . .
Si1 Si 0.6301(3) 0.29030(8) 0.2850(2) 0.1033(10) Uani 1 1 d . . .
C100 C 0.5218(12) 0.2304(3) 0.3389(7) 0.133(4) Uani 1 1 d . . .
H10G H 0.4087 0.2411 0.3556 0.200 Uiso 1 1 calc R . .
H10H H 0.5823 0.2187 0.3953 0.200 Uiso 1 1 calc R . .
H10I H 0.5175 0.1999 0.2941 0.200 Uiso 1 1 calc R . .
C101 C 0.8291(9) 0.2614(3) 0.2387(12) 0.206(8) Uani 1 1 d . . .
H10J H 0.8854 0.2403 0.2881 0.308 Uiso 1 1 calc R . .
H10K H 0.9009 0.2916 0.2185 0.308 Uiso 1 1 calc R . .
H10L H 0.8049 0.2373 0.1854 0.308 Uiso 1 1 calc R . .
C102 C 0.6877(11) 0.3379(3) 0.3819(7) 0.133(4) Uani 1 1 d . . .
H10M H 0.7476 0.3696 0.3566 0.200 Uiso 1 1 calc R . .
H10N H 0.7587 0.3186 0.4272 0.200 Uiso 1 1 calc R . .
H10O H 0.5870 0.3507 0.4131 0.200 Uiso 1 1 calc R . .

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N1 0.055(3) 0.044(3) 0.057(3) -0.001(3) 0.008(3) -0.003(2)
C1 0.048(3) 0.059(4) 0.049(4) -0.004(3) 0.009(3) -0.006(3)
Si2 0.1281(19) 0.0496(11) 0.0639(14) -0.0019(10) 0.0339(14) 0.0131(12)
N2 0.041(3) 0.049(3) 0.055(3) 0.009(3) 0.003(2) -0.003(2)
N3 0.047(3) 0.040(3) 0.051(3) 0.005(3) 0.012(2) 0.002(2)
N4 0.053(3) 0.046(3) 0.040(3) 0.002(2) 0.004(2) 0.002(2)
N5 0.053(3) 0.073(4) 0.043(3) -0.006(3) 0.010(3) -0.011(3)
N6 0.061(3) 0.066(3) 0.040(3) 0.006(3) 0.002(3) -0.019(3)
N7 0.057(3) 0.042(3) 0.078(4) 0.011(3) 0.010(3) 0.005(2)
C10 0.106(6) 0.055(4) 0.105(6) -0.016(5) -0.009(5) -0.022(4)
C11 0.073(4) 0.053(4) 0.050(4) 0.003(3) -0.003(4) -0.017(4)
C12 0.059(4) 0.066(4) 0.070(5) 0.011(4) 0.002(4) -0.022(4)
C13 0.042(3) 0.055(4) 0.073(5) 0.017(4) -0.002(3) -0.008(3)
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C14 0.056(4) 0.072(5) 0.126(7) 0.021(5) -0.004(5) 0.009(4)
C20 0.093(5) 0.049(4) 0.104(6) 0.012(4) 0.021(5) 0.018(4)
C21 0.055(4) 0.049(4) 0.065(5) 0.015(4) 0.014(3) 0.010(3)
C22 0.075(4) 0.067(5) 0.053(4) 0.023(4) 0.008(4) 0.017(4)
C23 0.052(3) 0.066(4) 0.045(4) 0.007(3) 0.010(3) 0.005(3)
C24 0.087(5) 0.080(5) 0.053(4) -0.004(4) -0.008(4) 0.013(4)
C30 0.107(6) 0.136(8) 0.085(6) -0.054(6) 0.033(5) 0.017(6)
C31 0.074(5) 0.130(7) 0.045(4) -0.020(5) 0.014(4) -0.006(5)
C32 0.069(5) 0.151(8) 0.052(5) 0.012(6) 0.020(4) -0.016(5)
C33 0.052(4) 0.107(6) 0.043(4) 0.022(4) 0.002(3) -0.022(4)
C34 0.075(5) 0.126(7) 0.078(6) 0.049(5) -0.008(4) -0.045(5)
C200 0.246(12) 0.105(7) 0.113(8) 0.036(6) 0.109(8) 0.074(8)
C201 0.127(7) 0.106(7) 0.089(6) -0.022(5) -0.014(6) -0.031(6)
C202 0.325(16) 0.051(5) 0.093(7) -0.009(5) -0.007(9) 0.009(7)
Si1 0.0683(13) 0.0492(12) 0.191(3) 0.0391(15) -0.0496(16) -0.0143(10)
C100 0.167(9) 0.078(6) 0.153(9) 0.061(6) -0.089(8) -0.054(6)
C101 0.062(5) 0.061(6) 0.49(3) 0.033(10) -0.023(9) 0.013(4)
C102 0.121(7) 0.092(6) 0.185(10) 0.065(7) -0.097(7) -0.057(5)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Zn1 N6 2.039(5) . ?
Zn1 N2 2.054(4) . ?
Zn1 N4 2.099(5) . ?
N1 C11 1.334(7) . ?
N1 N2 1.379(6) . ?
N1 C1 1.456(7) . ?
C1 N5 1.430(7) . ?
C1 N3 1.446(7) . ?
Si2 N7 1.684(6) . ?
Si2 C200 1.850(8) . ?
Si2 C201 1.861(9) . ?
Si2 C202 1.915(8) . ?
N2 C13 1.329(7) . ?
N3 C21 1.343(7) . ?
N3 N4 1.400(6) . ?
N4 C23 1.328(7) . ?
N5 C31 1.345(8) . ?
N5 N6 1.382(7) . ?
N6 C33 1.328(7) . ?
N7 Si1 1.693(5) . ?
C10 C11 1.508(9) . ?
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C10 H10B 0.9800 . ?
C10 H10C 0.9800 . ?
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C12 H12 0.9500 . ?
C13 C14 1.488(9) . ?
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C14 H14C 0.9800 . ?
C20 C21 1.477(9) . ?
C20 H20A 0.9800 . ?
C20 H20B 0.9800 . ?
C20 H20C 0.9800 . ?
C21 C22 1.348(9) . ?
C22 C23 1.387(8) . ?
C22 H22 0.9500 . ?
C23 C24 1.483(8) . ?
C24 H24A 0.9800 . ?
C24 H24B 0.9800 . ?
C24 H24C 0.9800 . ?
C30 C31 1.486(11) . ?
C30 H30A 0.9800 . ?
C30 H30B 0.9800 . ?
C30 H30C 0.9800 . ?
C31 C32 1.361(10) . ?
C32 C33 1.379(10) . ?
C32 H32 0.9500 . ?
C33 C34 1.477(10) . ?
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C34 H34B 0.9800 . ?
C34 H34C 0.9800 . ?
C200 H20G 0.9800 . ?
C200 H20H 0.9800 . ?
C200 H20I 0.9800 . ?
C201 H20J 0.9800 . ?
C201 H20K 0.9800 . ?
C201 H20L 0.9800 . ?
C202 H20M 0.9800 . ?
C202 H20N 0.9800 . ?
C202 H20O 0.9800 . ?
Si1 C102 1.862(10) . ?
Si1 C100 1.869(8) . ?
Si1 C101 1.879(10) . ?
C100 H10G 0.9800 . ?
C100 H10H 0.9800 . ?
C100 H10I 0.9800 . ?
C101 H10J 0.9800 . ?
C101 H10K 0.9800 . ?
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N7 Zn1 N2 123.72(19) . . ?
N6 Zn1 N2 92.86(19) . . ?
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N6 Zn1 N4 90.12(19) . . ?
N2 Zn1 N4 86.52(18) . . ?
C11 N1 N2 110.7(5) . . ?
C11 N1 C1 127.3(5) . . ?
N2 N1 C1 121.7(4) . . ?
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N5 C1 N3 109.6(5) . . ?
N5 C1 N1 110.4(5) . . ?
N3 C1 N1 109.1(5) . . ?
N7 Si2 C200 111.4(4) . . ?
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N7 Si2 C202 113.3(4) . . ?
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C13 N2 N1 105.5(5) . . ?
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C21 N3 C1 126.3(5) . . ?
N4 N3 C1 123.5(4) . . ?
C23 N4 N3 105.4(5) . . ?
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N6 N5 C1 122.0(5) . . ?
C33 N6 N5 105.8(6) . . ?
C33 N6 Zn1 141.0(5) . . ?
N5 N6 Zn1 112.8(3) . . ?
Si2 N7 Si1 123.7(3) . . ?
Si2 N7 Zn1 117.5(3) . . ?
Si1 N7 Zn1 118.7(3) . . ?
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C11 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
C11 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C11 C 0.1671(2) 0.8682(2) 0.28758(19) 0.0179(4) Uani 1 1 d . . .
C10 C 0.0844(2) 0.9477(2) 0.15307(19) 0.0236(4) Uani 1 1 d . . .
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H10B H 0.0323 1.0445 0.1490 0.035 Uiso 1 1 calc R . .
H10C H 0.0066 0.8883 0.1448 0.035 Uiso 1 1 calc R . .
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H20C H 0.2802 0.6148 -0.0270 0.045 Uiso 1 1 calc R . .
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C32 C 0.7460(2) 0.7301(2) 0.11321(19) 0.0216(4) Uani 1 1 d . . .
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H34B H 0.9529 0.6545 0.3409 0.039 Uiso 1 1 calc R . .
H34C H 0.9579 0.5032 0.3162 0.039 Uiso 1 1 calc R . .
C31 C 0.5914(2) 0.7624(2) 0.07812(18) 0.0183(4) Uani 1 1 d . . .
C30 C 0.5135(3) 0.8507(2) -0.05857(19) 0.0236(4) Uani 1 1 d . . .
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C22 0.0229(12) 0.0274(10) 0.0265(10) -0.0168(8) -0.0007(8) -0.0058(9)
C24 0.0335(14) 0.0202(10) 0.0305(11) -0.0079(8) -0.0040(9) -0.0071(9)
C13 0.0227(12) 0.0213(9) 0.0160(9) -0.0085(7) 0.0009(7) -0.0033(8)
C14 0.0364(14) 0.0275(10) 0.0161(9) -0.0106(8) -0.0005(8) 0.0022(9)
C23 0.0175(11) 0.0219(9) 0.0243(9) -0.0109(8) 0.0003(8) -0.0021(8)
C11 0.0156(11) 0.0185(9) 0.0186(9) -0.0060(7) -0.0013(7) -0.0013(7)
C10 0.0226(12) 0.0249(10) 0.0199(9) -0.0057(8) -0.0053(8) 0.0017(8)
C20 0.0388(15) 0.0333(11) 0.0209(10) -0.0126(9) -0.0080(9) -0.0072(10)
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C31 0.0203(12) 0.0198(9) 0.0157(8) -0.0078(7) 0.0020(8) -0.0032(8)
C30 0.0225(12) 0.0294(10) 0.0154(9) -0.0053(8) 0.0005(8) -0.0023(9)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C24 H24B 0.9800 . ?
C24 H24C 0.9800 . ?
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C14 H14A 0.9800 . ?
C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
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C10 H10A 0.9800 . ?
C10 H10B 0.9800 . ?
C10 H10C 0.9800 . ?
C20 H20A 0.9800 . ?
C20 H20B 0.9800 . ?
C20 H20C 0.9800 . ?
N6 C33 1.335(3) . ?
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C32 H32 0.9500 . ?
C34 H34A 0.9800 . ?
C34 H34B 0.9800 . ?
C34 H34C 0.9800 . ?
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N6 Zn1 N4 94.42(6) . 2_666 ?
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N6 Zn1 N4 85.58(6) . . ?
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C21 N3 C1 126.62(16) . . ?
N4 N3 C1 123.08(15) . . ?
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C31 N5 C1 126.77(16) . . ?
N6 N5 C1 122.79(14) . . ?
C23 N4 N3 106.11(15) . . ?
C23 N4 Zn1 138.14(13) . . ?
N3 N4 Zn1 114.88(11) . . ?
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C11 N1 C1 126.13(15) . . ?
N2 N1 C1 123.60(15) . . ?
C11 C12 C13 106.44(17) . . ?
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C13 C12 H12 126.8 . . ?
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N5 C1 N1 109.62(15) . . ?
N3 C1 N1 109.15(14) . . ?
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C23 C24 H24B 109.5 . . ?
H24A C24 H24B 109.5 . . ?
C23 C24 H24C 109.5 . . ?
H24A C24 H24C 109.5 . . ?
H24B C24 H24C 109.5 . . ?
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N2 C13 C14 121.15(18) . . ?
C12 C13 C14 128.75(18) . . ?
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C13 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
C13 C14 H14C 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
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N1 C11 C10 122.49(17) . . ?
C12 C11 C10 130.08(18) . . ?
C11 C10 H10A 109.5 . . ?
C11 C10 H10B 109.5 . . ?
H10A C10 H10B 109.5 . . ?
C11 C10 H10C 109.5 . . ?
H10A C10 H10C 109.5 . . ?
H10B C10 H10C 109.5 . . ?
C21 C20 H20A 109.5 . . ?
C21 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C21 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
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C33 N6 Zn1 137.99(13) . . ?
N5 N6 Zn1 115.83(11) . . ?
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N6 C33 C34 121.31(17) . . ?
C32 C33 C34 128.97(19) . . ?
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C31 C32 H32 126.7 . . ?
C33 C32 H32 126.7 . . ?
C33 C34 H34A 109.5 . . ?
C33 C34 H34B 109.5 . . ?
H34A C34 H34B 109.5 . . ?
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N5 C31 C30 122.15(18) . . ?
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C31 C30 H30A 109.5 . . ?
C31 C30 H30B 109.5 . . ?
H30A C30 H30B 109.5 . . ?
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N6 Zn1 N2 N1 -134.41(12) 2_666 . . . ?
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C1 N3 N4 C23 -179.78(16) . . . . ?
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C13 N2 N1 C11 -0.1(2) . . . . ?
Zn1 N2 N1 C11 175.18(12) . . . . ?
C13 N2 N1 C1 179.13(16) . . . . ?
Zn1 N2 N1 C1 -5.6(2) . . . . ?
C31 N5 C1 N3 116.97(18) . . . . ?
N6 N5 C1 N3 -59.3(2) . . . . ?
C31 N5 C1 N1 -123.87(18) . . . . ?
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N4 N3 C1 N1 -53.4(2) . . . . ?
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N2 N1 C1 N5 -55.6(2) . . . . ?
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N4 N3 C21 C22 1.1(2) . . . . ?
C1 N3 C21 C22 179.46(18) . . . . ?
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C1 N3 C21 C20 0.2(3) . . . . ?
N3 C21 C22 C23 -0.4(2) . . . . ?
C20 C21 C22 C23 178.8(2) . . . . ?
N1 N2 C13 C12 -0.1(2) . . . . ?
Zn1 N2 C13 C12 -173.71(15) . . . . ?
N1 N2 C13 C14 179.66(17) . . . . ?
Zn1 N2 C13 C14 6.1(3) . . . . ?
C11 C12 C13 N2 0.4(2) . . . . ?
C11 C12 C13 C14 -179.4(2) . . . . ?
N3 N4 C23 C22 1.1(2) . . . . ?
Zn1 N4 C23 C22 -167.08(15) . . . . ?
N3 N4 C23 C24 -178.52(18) . . . . ?
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C21 C22 C23 N4 -0.4(2) . . . . ?
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N2 N1 C11 C12 0.4(2) . . . . ?
C1 N1 C11 C12 -178.87(17) . . . . ?
N2 N1 C11 C10 -177.70(17) . . . . ?
C1 N1 C11 C10 3.1(3) . . . . ?
C13 C12 C11 N1 -0.4(2) . . . . ?
C13 C12 C11 C10 177.43(19) . . . . ?
C31 N5 N6 C33 0.5(2) . . . . ?
C1 N5 N6 C33 177.37(15) . . . . ?
C31 N5 N6 Zn1 -178.62(11) . . . . ?
C1 N5 N6 Zn1 -1.8(2) . . . . ?
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N4 Zn1 N6 N5 42.32(12) . . . . ?
N5 N6 C33 C32 -0.5(2) . . . . ?
Zn1 N6 C33 C32 178.39(14) . . . . ?
N5 N6 C33 C34 179.43(17) . . . . ?
Zn1 N6 C33 C34 -1.7(3) . . . . ?
N6 C33 C32 C31 0.2(2) . . . . ?
C34 C33 C32 C31 -179.6(2) . . . . ?
N6 N5 C31 C32 -0.4(2) . . . . ?
C1 N5 C31 C32 -177.07(17) . . . . ?
N6 N5 C31 C30 178.70(16) . . . . ?
C1 N5 C31 C30 2.0(3) . . . . ?
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Table 1. Crystal data and structure refinement for Mg{C(Me2pz)3}{C(pz)3} (**MGC26**)

Empirical formula	C26 H30 Mg N12
Formula weight	534.91
Crystal description	orange plate
Crystal size	0.25 x 0.20 x 0.10 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	C 1 2/m 1
Unit cell dimensions	a = 35.6839(11) A alpha = 90 deg. b = 13.3948(4) A beta = 94.3134(15) deg. c = 8.0750(3) A gamma = 90 deg.
Reflections for cell refinement	3878
Range in theta	5 to 26 deg.
Volume, Z	3848.7(2) A^3, 4
Density (calculated)	0.923 Mg/m^3
Absorption coefficient	0.075 mm^-1
F(000)	1128
Diffractometer type	Area
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.107 to 26.055 deg.
Index ranges	-44<=h<=43, 0<=k<=16, 0<=l<=9
Reflections collected	3929
Independent reflections	3929 [R(merge) = 0.037]
Observed reflections	2762 [I>2sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.99, Tmax = 0.99)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Geometric
Hydrogen atom treatment	Riding model
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev polynomial
Data / restraints / parameters	2762 / 283/ 205

Goodness-of-fit on F	0.9881
Final R indices [I>3sigma(I)]	R1 = 0.0787, Rw = 0.0817
Final maximum delta/sigma	0.0012
Largest diff. peak and hole	0.46 and -0.30 e.A^-3

Comments

Molecules of MGC26 lie across crystallographic mirror planes. The difference map indicated the presence of diffuse electron density believed to be disordered solvent. It was not possible to model this residual density conventionally. SQUEEZE was used leaving a void from which the electron density was removed.

The discrete Fourier transform of the void region were treated as contributions to the A and B parts of the calculated structure factors.

H atoms were placed in calculated positions and refined in a riding model. The orientation of the methyl groups was confirmed by reference to a Fourier difference map.

Soft similarity restraints were applied to the displacement parameters

Table 2. Selected bond lengths [A] and angles [deg] for MGC26.

Mg(1)-N(1)	2.186(3)
Mg(1)-N(3)	2.1609(19)
Mg(1)-N(5)	2.197(3)
Mg(1)-N(7)	2.177(2)
Mg(1)-N(3A)	2.1609(19)
Mg(1)-N(7A)	2.177(2)
N(1)-C(1)	1.329(4)
N(1)-N(2)	1.380(4)
C(1)-C(2)	1.410(5)
C(1)-C(4)	1.485(5)
N(2)-C(3)	1.360(4)
N(2)-C(11)	1.442(4)
C(2)-C(3)	1.371(5)
N(3)-N(4)	1.384(2)
N(3)-C(6)	1.336(3)
C(3)-C(5)	1.481(5)
N(4)-C(8)	1.356(3)
N(4)-C(11)	1.450(3)
N(5)-N(6)	1.379(3)
N(5)-C(12)	1.319(4)
N(6)-C(14)	1.347(4)
N(6)-C(18)	1.448(4)
C(6)-C(7)	1.398(3)
C(6)-C(9)	1.490(4)
N(7)-N(8)	1.376(3)
N(7)-C(15)	1.333(3)
C(7)-C(8)	1.373(4)
N(8)-C(17)	1.349(3)
N(8)-C(18)	1.451(3)
C(8)-C(10)	1.499(3)
C(12)-C(13)	1.389(5)
C(13)-C(14)	1.362(5)
C(15)-C(16)	1.391(4)
C(16)-C(17)	1.365(4)
N(3A) -Mg(1)-N(7A)	96.14(7)
N(3A) -Mg(1)-N(1)	85.03(7)
N(7A) -Mg(1)-N(1)	94.52(8)
N(3A) -Mg(1)-N(3)	84.40(10)
N(7A) -Mg(1)-N(3)	179.27(9)
N(1)-Mg(1)-N(3)	85.03(7)
N(3A) -Mg(1)-N(5)	97.90(8)
N(7A) -Mg(1)-N(5)	82.52(8)
N(1)-Mg(1)-N(5)	176.02(10)
N(3)-Mg(1)-N(5)	97.90(8)
N(3A) -Mg(1)-N(7)	179.27(9)
N(7A) -Mg(1)-N(7)	83.31(11)
N(1)-Mg(1)-N(7)	94.52(8)
N(3)-Mg(1)-N(7)	96.14(7)
N(5)-Mg(1)-N(7)	82.52(8)
Mg(1)-N(1)-C(1)	138.6(2)
Mg(1)-N(1)-N(2)	114.92(19)
C(1)-N(1)-N(2)	106.5(3)
N(1)-C(1)-C(2)	109.6(3)
N(1)-C(1)-C(4)	122.3(3)
C(2)-C(1)-C(4)	128.1(3)
N(1)-N(2)-C(3)	110.4(3)
N(1)-N(2)-C(11)	123.6(2)
C(3)-N(2)-C(11)	126.1(3)
C(1)-C(2)-C(3)	106.7(3)

Mg(1)-N(3)-N(4)	115.17(14)
Mg(1)-N(3)-C(6)	138.88(16)
N(4)-N(3)-C(6)	105.82(18)
C(2)-C(3)-N(2)	106.9(3)
C(2)-C(3)-C(5)	131.4(3)
N(2)-C(3)-C(5)	121.7(3)
N(3)-N(4)-C(8)	110.16(19)
N(3)-N(4)-C(11)	123.64(19)
C(8)-N(4)-C(11)	126.2(2)
Mg(1)-N(5)-N(6)	116.55(19)
Mg(1)-N(5)-C(12)	138.1(2)
N(6)-N(5)-C(12)	105.3(2)
N(5)-N(6)-C(14)	110.0(3)
N(5)-N(6)-C(18)	124.2(2)
C(14)-N(6)-C(18)	125.8(3)
N(3)-C(6)-C(7)	110.4(2)
N(3)-C(6)-C(9)	121.5(2)
C(7)-C(6)-C(9)	128.1(2)
Mg(1)-N(7)-N(8)	117.43(14)
Mg(1)-N(7)-C(15)	137.50(17)
N(8)-N(7)-C(15)	105.00(19)
C(6)-C(7)-C(8)	106.2(2)
N(7)-N(8)-C(17)	110.02(19)
N(7)-N(8)-C(18)	123.77(19)
C(17)-N(8)-C(18)	126.2(2)
C(7)-C(8)-N(4)	107.4(2)
C(7)-C(8)-C(10)	129.7(2)
N(4)-C(8)-C(10)	122.8(2)
N(4A) -C(11)-N(4)	109.9(2)
N(4A) -C(11)-N(2)	108.64(17)
N(4)-C(11)-N(2)	108.64(17)
N(5)-C(12)-C(13)	111.4(3)
C(12)-C(13)-C(14)	105.3(3)
C(13)-C(14)-N(6)	108.0(3)
N(7)-C(15)-C(16)	111.7(2)
C(15)-C(16)-C(17)	104.7(2)
C(16)-C(17)-N(8)	108.5(2)
N(8)-C(18)-N(8A)	107.6(2)
N(8)-C(18)-N(6)	108.29(16)
N(8A) -C(18)-N(6)	108.29(16)

Atoms carrying the suffix 'A' are related to their couterparts by
The symmetry operator x,-y,z

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data_MGC46
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No special comments
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 H       0.0000   0.0000   0.4930  10.5109   0.3229  26.1257   0.1402   3.1424
   0.0408  57.7998   0.0030 'International Tables Vol C 4.2.6.8 and 6.1.1.4'
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_reflns_limit_l_min               0
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# The current dictionary definitions do not cover the
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# selected by a user-defined sigma threshold


# The values actually used during refinement
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_refine_ls_number_parameters     199
_oxford_refine_ls_R_factor_ref   0.0504
_refine_ls_wR_factor_ref         0.0541
_refine_ls_goodness_of_fit_ref   1.0880
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# The values computed from all data
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# The values computed with a 2 sigma cutoff - a la SHELX
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_refine_ls_wR_factor_gt          0.0565

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_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 1.63 1.32 1.50 0.386 0.350
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C.,
Polidori, G. & Camalli, M. (1994). J. Appl. Cryst. 27, 435.

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Prout, K. & Watkin, D.J. (2003). J. Appl. Cryst. 36, 1487.

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and Materials Science
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Watkin, D.J., Prout, C.K. & Pearce, L.J. (1996). CAMERON, Chemical
Crystallography Laboratory, Oxford, UK.
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Uequiv = arithmetic mean of Ui i.e. Ueqiv = (U1+U2+U3)/3

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_atom_site_adp_type
_atom_site_refinement_flags_posn
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C2 C 0.24240(10) -0.08464(19) 0.07816(18) 0.0321 1.0000 Uani . . . . . .
C3 C 0.26566(10) 0.04778(18) 0.12487(17) 0.0298 1.0000 Uani . . . . . .
C4 C 0.27247(13) -0.1702(2) -0.0354(2) 0.0442 1.0000 Uani . . . . . .
C5 C 0.29703(14) -0.3195(2) 0.0083(3) 0.0550 1.0000 Uani . . . . . .
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C8 C 0.33314(11) 0.3707(2) 0.2466(2) 0.0366 1.0000 Uani . . . . . .
C9 C 0.46664(13) 0.4792(3) 0.2459(4) 0.0678 1.0000 Uani . . . . . .
C10 C 0.54425(15) 0.4251(4) 0.2619(5) 0.0999 1.0000 Uani . . . . . .
C11 C 0.11530(10) 0.45490(19) 0.10148(18) 0.0302 1.0000 Uani . . . . . .
C12 C 0.08599(9) 0.48871(18) 0.22623(18) 0.0288 1.0000 Uani . . . . . .
C13 C 0.12335(9) 0.39814(18) 0.32020(17) 0.0279 1.0000 Uani . . . . . .
C14 C 0.02458(10) 0.5953(2) 0.2486(2) 0.0377 1.0000 Uani . . . . . .
C15 C 0.03620(13) 0.6744(2) 0.3847(2) 0.0481 1.0000 Uani . . . . . .
C16 C 0.22493(9) 0.21254(18) 0.30990(17) 0.0279 1.0000 Uani . . . . . .
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N5 N 0.16670(8) 0.35069(16) 0.11484(14) 0.0315 1.0000 Uani . . . . . .
N6 N 0.17059(8) 0.31662(15) 0.25069(14) 0.0275 1.0000 Uani . . . . . .
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H31 H 0.3045 0.1044 0.0910 0.0383 1.0000 Uiso R . . . . . .
H41 H 0.3149 -0.1212 -0.0656 0.0555 1.0000 Uiso R . . . . . .
H42 H 0.2338 -0.1773 -0.1096 0.0555 1.0000 Uiso R . . . . . .
H51 H 0.3156 -0.3696 -0.0665 0.0711 1.0000 Uiso R . . . . . .
H52 H 0.3359 -0.3132 0.0822 0.0711 1.0000 Uiso R . . . . . .

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H53 H 0.2547 -0.3693 0.0382 0.0711 1.0000 Uiso R . . . . . .
H61 H 0.4614 0.2661 0.4617 0.0553 1.0000 Uiso R . . . . . .
H81 H 0.3086 0.4228 0.1713 0.0460 1.0000 Uiso R . . . . . .
H91 H 0.4659 0.5671 0.2949 0.0869 1.0000 Uiso R . . . . . .
H92 H 0.4530 0.4962 0.1506 0.0869 1.0000 Uiso R . . . . . .
H101 H 0.5779 0.4922 0.2269 0.1298 1.0000 Uiso R . . . . . .
H102 H 0.5589 0.4085 0.3569 0.1298 1.0000 Uiso R . . . . . .
H103 H 0.5461 0.3376 0.2125 0.1298 1.0000 Uiso R . . . . . .
H111 H 0.1004 0.5016 0.0165 0.0381 1.0000 Uiso R . . . . . .
H131 H 0.1177 0.3934 0.4161 0.0356 1.0000 Uiso R . . . . . .
H141 H 0.0231 0.6640 0.1764 0.0470 1.0000 Uiso R . . . . . .
H142 H -0.0226 0.5462 0.2447 0.0470 1.0000 Uiso R . . . . . .
H151 H -0.0042 0.7401 0.3921 0.0601 1.0000 Uiso R . . . . . .
H152 H 0.0830 0.7250 0.3898 0.0601 1.0000 Uiso R . . . . . .
H153 H 0.0373 0.6071 0.4580 0.0601 1.0000 Uiso R . . . . . .
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C9 0.0410(12) 0.0441(13) 0.117(2) 0.0116(14) 0.0033(13) -0.0084(10)
C10 0.0438(15) 0.074(2) 0.183(4) 0.039(2) 0.0173(18) -0.0075(14)
C11 0.0312(8) 0.0316(9) 0.0276(8) 0.0025(7) 0.0017(7) -0.0008(7)
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C13 0.0265(8) 0.0332(8) 0.0248(8) -0.0034(6) 0.0058(6) -0.0005(7)
C14 0.0300(9) 0.0448(11) 0.0380(10) -0.0004(8) 0.0014(7) 0.0087(8)
C15 0.0524(12) 0.0481(12) 0.0437(11) -0.0049(9) 0.0045(9) 0.0211(10)
C16 0.0306(8) 0.0295(8) 0.0240(8) 0.0006(6) 0.0051(6) 0.0027(7)
N1 0.0323(8) 0.0360(8) 0.0386(8) 0.0033(7) 0.0057(6) -0.0066(6)
N2 0.0302(7) 0.0277(7) 0.0288(7) 0.0024(6) 0.0049(6) 0.0003(6)
N3 0.0351(8) 0.0496(10) 0.0335(8) 0.0012(7) 0.0017(6) 0.0101(7)
N4 0.0304(7) 0.0331(8) 0.0259(7) -0.0021(6) 0.0025(6) 0.0027(6)
N5 0.0357(8) 0.0355(8) 0.0238(7) 0.0018(6) 0.0049(6) 0.0019(6)
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C15 . H153 . 0.950    no
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C16 . N6 . 1.449(2)    yes
C16 . H161 . 0.950    no
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N1 . C1 . H11 . 123.5    no
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C1 . C2 . C4 . 128.77(17)    yes
C3 . C2 . C4 . 127.55(17)    yes
C2 . C3 . N2 . 107.41(15)    yes
C2 . C3 . H31 . 126.3    no
N2 . C3 . H31 . 126.3    no
C2 . C4 . C5 . 113.36(18)    yes
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C2 . C4 . H41 . 108.5    no
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H41 . C4 . H42 . 109.5    no
C4 . C5 . H51 . 110.5    no
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H51 . C5 . H52 . 109.5    no
C4 . C5 . H53 . 108.9    no
H51 . C5 . H53 . 109.5    no
H52 . C5 . H53 . 109.5    no
C7 . C6 . N3 . 113.27(18)    yes
C7 . C6 . H61 . 123.2    no
N3 . C6 . H61 . 123.6    no
C6 . C7 . C8 . 103.83(18)    yes
C6 . C7 . C9 . 129.6(2)    yes
C8 . C7 . C9 . 126.6(2)    yes
C7 . C8 . N4 . 106.97(17)    yes
C7 . C8 . H81 . 126.5    no
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H102 . C10 . H103 . 109.5    no
C12 . C11 . N5 . 112.69(15)    yes
C12 . C11 . H111 . 123.8    no
N5 . C11 . H111 . 123.5    no
C11 . C12 . C13 . 104.19(15)    yes
C11 . C12 . C14 . 127.29(16)    yes
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C12 . C13 . N6 . 107.12(14)    yes
C12 . C13 . H131 . 126.6    no
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C1 . N1 . N2 . 103.39(14)    yes
C16 . N2 . N1 . 118.49(14)    yes
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C16	N2	C3 . 129.11(14) yes
N1	N2	C3 . 112.38(14) yes
C6	N3	N4 . 103.16(16) yes
C16	N4	C8 . 129.96(15) yes
C16	N4	N3 . 117.08(14) yes
C8	N4	N3 . 112.76(15) yes
C11	N5	N6 . 103.79(13) yes
C16	N6	C13 . 126.51(14) yes
C16	N6	N5 . 121.09(13) yes
C13	N6	N5 . 112.20(14) yes

Table 1. Crystal data and structure refinement for Mg{(tBu2pz)2CHSiMe2NiPr}({N(SiMe3)2} (mg7).

Empirical formula	C37 H68 Mg1 N6 Si3
Formula weight	705.55
Crystal description	white block
Crystal size	0.20 x 0.20 x 0.20 mm
Temperature	150 K
Crystal system	Orthorhombic
Space group	P 21 21 21
Unit cell dimensions	a = 13.9372(2) A alpha = 90 deg. b = 15.2750(2) A beta = 90 deg. c = 20.1552(2) A gamma = 90 deg.
Reflections for cell refinement	5381
Range in theta	5 to 27 deg.
Volume, Z	4290.85(9) A^3, 4
Density (calculated)	1.092 Mg/m^3
Absorption coefficient	0.157 mm^-1
F(000)	1544
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.137 to 27.483 deg.
Index ranges	0<=h<=18, 0<=k<=19, 0<=l<=26
Reflections collected	9765
Independent reflections	5371 [R(merge) = 0.022]
Observed reflections	4450 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.97, Tmax = 0.97)

Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Geometric
Hydrogen atom treatment	Riding
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev
Data / restraints / parameters	4450 / 0/ 424
Goodness-of-fit on F	1.1189
Final R indices [I>3sigma(I)]	R1 = 0.0357, Rw = 0.0372
Final maximum delta/sigma	0.0006
Largest diff. peak and hole	0.25 and -0.24 e.A^-3

Comments:
In the absence of heavy atoms Friedel pairs were merged and a Flack paramater was not estimated. For light atoms the differences in anomalous scattering may be ignored

Table 2. Selected bond lengths [A] and angles [deg] for mg7.

Mg(1)-N(1)	2.254(2)
Mg(1)-N(3)	2.206(2)
Mg(1)-N(5)	2.023(2)
Mg(1)-N(6)	2.023(2)
N(1)-N(2)	1.377(3)
N(1)-C(1)	1.359(3)
N(2)-C(3)	1.367(3)
N(2)-C(23)	1.472(3)
N(3)-N(4)	1.399(3)
N(3)-C(12)	1.337(3)
N(4)-C(14)	1.379(3)
N(4)-C(23)	1.469(3)
N(5)-Si(1)	1.685(2)
N(5)-C(26)	1.402(3)
N(6)-Si(2)	1.712(2)
N(6)-Si(3)	1.706(2)
Si(1)-C(23)	1.959(2)
Si(1)-C(24)	1.875(3)
Si(1)-C(25)	1.877(3)
Si(2)-C(32)	1.877(3)
Si(2)-C(33)	1.880(3)
Si(2)-C(34)	1.886(3)
Si(3)-C(35)	1.890(3)
Si(3)-C(36)	1.888(3)
Si(3)-C(37)	1.885(3)
C(1)-C(2)	1.387(3)
C(1)-C(4)	1.515(3)
C(2)-C(3)	1.385(3)
C(3)-C(8)	1.535(3)
C(4)-C(5)	1.536(3)
C(4)-C(6)	1.539(3)
C(4)-C(7)	1.543(3)
C(8)-C(9)	1.552(4)
C(8)-C(10)	1.532(4)
C(8)-C(11)	1.540(4)
C(12)-C(13)	1.405(3)
C(12)-C(15)	1.514(3)
C(13)-C(14)	1.372(4)
C(14)-C(19)	1.511(3)
C(15)-C(16)	1.516(4)
C(15)-C(17)	1.532(4)
C(15)-C(18)	1.546(4)
C(19)-C(20)	1.533(4)
C(19)-C(21)	1.544(4)
C(19)-C(22)	1.532(4)
C(26)-C(27)	1.403(4)
C(26)-C(31)	1.397(4)
C(27)-C(28)	1.390(4)
C(28)-C(29)	1.382(4)
C(29)-C(30)	1.385(4)
C(30)-C(31)	1.394(4)

N(1)-Mg(1)-N(3)	91.70(7)
N(1)-Mg(1)-N(5)	92.76(8)
N(3)-Mg(1)-N(5)	92.00(8)
N(1)-Mg(1)-N(6)	123.88(8)
N(3)-Mg(1)-N(6)	116.93(8)
N(5)-Mg(1)-N(6)	129.76(8)
Mg(1)-N(1)-N(2)	113.34(13)
Mg(1)-N(1)-C(1)	137.81(15)

N(2)-N(1)-C(1)	105.02(17)
N(1)-N(2)-C(3)	111.97(17)
N(1)-N(2)-C(23)	117.09(17)
C(3)-N(2)-C(23)	130.66(19)
Mg(1)-N(3)-N(4)	108.81(13)
Mg(1)-N(3)-C(12)	141.07(16)
N(4)-N(3)-C(12)	106.06(18)
N(3)-N(4)-C(14)	109.91(18)
N(3)-N(4)-C(23)	114.71(17)
C(14)-N(4)-C(23)	130.17(19)
Mg(1)-N(5)-Si(1)	110.77(10)
Mg(1)-N(5)-C(26)	131.05(16)
Si(1)-N(5)-C(26)	118.13(16)
Mg(1)-N(6)-Si(2)	118.96(11)
Mg(1)-N(6)-Si(3)	118.11(11)
Si(2)-N(6)-Si(3)	122.93(12)
N(5)-Si(1)-C(23)	106.59(10)
N(5)-Si(1)-C(24)	112.10(12)
C(23)-Si(1)-C(24)	106.65(11)
N(5)-Si(1)-C(25)	118.69(11)
C(23)-Si(1)-C(25)	104.21(11)
C(24)-Si(1)-C(25)	107.70(13)
N(6)-Si(2)-C(32)	112.47(12)
N(6)-Si(2)-C(33)	112.34(12)
C(32)-Si(2)-C(33)	107.41(14)
N(6)-Si(2)-C(34)	114.78(12)
C(32)-Si(2)-C(34)	105.17(16)
C(33)-Si(2)-C(34)	103.95(15)
N(6)-Si(3)-C(35)	113.19(11)
N(6)-Si(3)-C(36)	115.78(12)
C(35)-Si(3)-C(36)	103.96(12)
N(6)-Si(3)-C(37)	109.76(11)
C(35)-Si(3)-C(37)	109.80(13)
C(36)-Si(3)-C(37)	103.79(13)
N(1)-C(1)-C(2)	109.8(2)
N(1)-C(1)-C(4)	124.6(2)
C(2)-C(1)-C(4)	125.6(2)
C(1)-C(2)-C(3)	108.0(2)
C(2)-C(3)-N(2)	105.22(19)
C(2)-C(3)-C(8)	122.2(2)
N(2)-C(3)-C(8)	132.5(2)
C(1)-C(4)-C(5)	111.32(19)
C(1)-C(4)-C(6)	109.2(2)
C(5)-C(4)-C(6)	111.0(2)
C(1)-C(4)-C(7)	109.5(2)
C(5)-C(4)-C(7)	108.4(2)
C(6)-C(4)-C(7)	107.4(2)
C(3)-C(8)-C(9)	106.8(2)
C(3)-C(8)-C(10)	118.1(2)
C(9)-C(8)-C(10)	107.1(2)
C(3)-C(8)-C(11)	107.9(2)
C(9)-C(8)-C(11)	108.2(2)
C(10)-C(8)-C(11)	108.3(2)
N(3)-C(12)-C(13)	110.0(2)
N(3)-C(12)-C(15)	123.8(2)
C(13)-C(12)-C(15)	125.8(2)
C(12)-C(13)-C(14)	107.4(2)
N(4)-C(14)-C(13)	106.5(2)
N(4)-C(14)-C(19)	125.7(2)
C(13)-C(14)-C(19)	127.7(2)
C(12)-C(15)-C(16)	111.8(2)
C(12)-C(15)-C(17)	109.9(2)
C(16)-C(15)-C(17)	110.9(2)
C(12)-C(15)-C(18)	106.7(2)

C(16)-C(15)-C(18)	108.8(2)
C(17)-C(15)-C(18)	108.7(2)
C(14)-C(19)-C(20)	110.4(2)
C(14)-C(19)-C(21)	110.0(2)
C(20)-C(19)-C(21)	112.2(2)
C(14)-C(19)-C(22)	109.2(2)
C(20)-C(19)-C(22)	107.9(2)
C(21)-C(19)-C(22)	107.1(2)
N(2)-C(23)-N(4)	112.29(18)
N(2)-C(23)-Si(1)	113.15(15)
N(4)-C(23)-Si(1)	110.78(15)
N(5)-C(26)-C(27)	122.3(2)
N(5)-C(26)-C(31)	121.1(2)
C(27)-C(26)-C(31)	116.6(2)
C(26)-C(27)-C(28)	121.8(3)
C(27)-C(28)-C(29)	120.8(3)
C(28)-C(29)-C(30)	118.4(3)
C(29)-C(30)-C(31)	121.1(3)
C(26)-C(31)-C(30)	121.3(3)

Table 1. Crystal data and structure refinement for Mg{(tBu2pz)2CHSiMe2NPh}({N(SiHMe2)2} . 0.75 C5H12 (mgc9)

Empirical formula	C35 H64 Mg1 N6 Si3 , 0.75 (C5 H12)
Formula weight	731.61
Crystal description	colourless plate
Crystal size	0.30 x 0.20 x 0.20 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a = 19.7490(9) A alpha = 90 deg. b = 11.0055(5) A beta = 110.253(2) deg. c = 22.6313(10) A gamma = 90 deg.
Reflections for cell refinement	9050
Range in theta	5 to 27 deg.
Volume, Z	4614.7(4) A^3, 4
Density (calculated)	1.053 Mg/m^3
Absorption coefficient	0.148 mm^-1
F(000)	1606
Diffractometer type	Nonius KappaCCD
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.132 to 27.431 deg.

Index ranges	-25<=h<=23, 0<=k<=14, 0<=l<=29
Reflections collected	31102
Independent reflections	10257 [R(merge) = 0.116]
Observed reflections	4225 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.75, Tmax = 0.97)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	Mixed
Hydrogen atom treatment	Mixed
Refinement method	Full-matrix least-squares on F
Weighting scheme	Chebychev polynomial
Data / restraints / parameters	4225 / 31/ 459
Goodness-of-fit on F	1.1389
Final R indices [I>3sigma(I)]	R1 = 0.0619, Rw = 0.0591
Final maximum delta/sigma	0.000204
Largest diff. peak and hole	0.85 and -0.41 e.A^-3

Comments:
Crystals of MGC9 contained a partial occupancy pentane of crystallization. This was refined anisotropically subject to loose similarity restraints for the C-C distances and angles, and the displacement parameters. Si-bound H atoms were located from a Fourier map and refined isotropically

Table 2. Selected bond lengths [A] and angles [deg] for mgc9.

Mg(1)-N(1)	2.167(4)
Mg(1)-N(3)	2.217(4)
Mg(1)-N(5)	2.027(4)
Mg(1)-N(6)	2.002(4)
N(1)-N(2)	1.390(5)
N(1)-C(1)	1.336(5)
N(2)-C(3)	1.381(5)
N(2)-C(23)	1.474(5)
N(3)-N(4)	1.391(5)
N(3)-C(12)	1.353(5)
N(4)-C(14)	1.373(5)
N(4)-C(23)	1.478(5)
N(5)-Si(1)	1.697(4)
N(5)-C(26)	1.392(5)
N(6)-Si(2)	1.700(4)
N(6)-Si(3)	1.705(4)
Si(1)-C(23)	1.956(5)
Si(1)-C(24)	1.866(5)
Si(1)-C(25)	1.855(4)
Si(2)-C(32)	1.861(5)
Si(2)-C(33)	1.879(5)
Si(2)-H(1)	1.43(4)
Si(3)-C(34)	1.865(5)
Si(3)-C(35)	1.862(5)
Si(3)-H(2)	1.39(4)
C(1)-C(2)	1.396(7)
C(1)-C(4)	1.505(6)
C(2)-C(3)	1.378(6)
C(3)-C(8)	1.505(6)
C(4)-C(5)	1.548(7)
C(4)-C(6)	1.536(7)
C(4)-C(7)	1.532(7)
C(8)-C(9)	1.540(7)
C(8)-C(10)	1.543(7)
C(8)-C(11)	1.541(7)
C(12)-C(13)	1.388(6)
C(12)-C(15)	1.514(6)
C(13)-C(14)	1.373(6)
C(14)-C(19)	1.548(6)
C(15)-C(16)	1.528(6)
C(15)-C(17)	1.530(7)
C(15)-C(18)	1.525(6)
C(19)-C(20)	1.561(6)
C(19)-C(21)	1.536(7)
C(19)-C(22)	1.519(7)
C(26)-C(27)	1.415(6)
C(26)-C(31)	1.394(6)
C(27)-C(28)	1.392(6)
C(28)-C(29)	1.383(7)
C(29)-C(30)	1.400(7)
C(30)-C(31)	1.393(6)
C(101)-C(102)	1.532(5)
C(102)-C(103)	1.534(5)
C(103)-C(104)	1.532(5)
C(104)-C(105)	1.530(5)
N(1)-Mg(1)-N(3)	96.03(14)
N(1)-Mg(1)-N(5)	91.87(15)
N(3)-Mg(1)-N(5)	92.54(14)
N(1)-Mg(1)-N(6)	109.39(15)

N(3)-Mg(1)-N(6)	119.10(15)
N(5)-Mg(1)-N(6)	138.33(16)
Mg(1)-N(1)-N(2)	107.0(2)
Mg(1)-N(1)-C(1)	139.5(3)
N(2)-N(1)-C(1)	106.2(3)
N(1)-N(2)-C(3)	110.2(3)
N(1)-N(2)-C(23)	113.0(3)
C(3)-N(2)-C(23)	132.3(4)
Mg(1)-N(3)-N(4)	113.5(2)
Mg(1)-N(3)-C(12)	138.4(3)
N(4)-N(3)-C(12)	105.0(3)
N(3)-N(4)-C(14)	111.1(3)
N(3)-N(4)-C(23)	115.7(3)
C(14)-N(4)-C(23)	132.0(4)
Mg(1)-N(5)-Si(1)	108.24(18)
Mg(1)-N(5)-C(26)	127.2(3)
Si(1)-N(5)-C(26)	123.5(3)
Mg(1)-N(6)-Si(2)	118.27(19)
Mg(1)-N(6)-Si(3)	121.1(2)
Si(2)-N(6)-Si(3)	120.6(2)
N(5)-Si(1)-C(23)	107.87(18)
N(5)-Si(1)-C(24)	118.0(2)
C(23)-Si(1)-C(24)	104.8(2)
N(5)-Si(1)-C(25)	114.7(2)
C(23)-Si(1)-C(25)	102.1(2)
C(24)-Si(1)-C(25)	107.7(2)
N(6)-Si(2)-C(32)	114.2(2)
N(6)-Si(2)-C(33)	113.1(2)
C(32)-Si(2)-C(33)	107.5(3)
N(6)-Si(3)-C(34)	111.6(2)
N(6)-Si(3)-C(35)	113.7(2)
C(34)-Si(3)-C(35)	109.8(3)
N(1)-C(1)-C(2)	110.0(4)
N(1)-C(1)-C(4)	124.2(4)
C(2)-C(1)-C(4)	125.7(4)
C(1)-C(2)-C(3)	107.7(4)
N(2)-C(3)-C(2)	105.9(4)
N(2)-C(3)-C(8)	125.8(4)
C(2)-C(3)-C(8)	128.3(4)
C(1)-C(4)-C(5)	106.4(4)
C(1)-C(4)-C(6)	111.4(4)
C(5)-C(4)-C(6)	108.8(5)
C(1)-C(4)-C(7)	110.7(4)
C(5)-C(4)-C(7)	109.5(4)
C(6)-C(4)-C(7)	110.0(5)
C(3)-C(8)-C(9)	110.5(4)
C(3)-C(8)-C(10)	108.4(4)
C(9)-C(8)-C(10)	108.0(4)
C(3)-C(8)-C(11)	109.8(4)
C(9)-C(8)-C(11)	112.7(4)
C(10)-C(8)-C(11)	107.3(4)
N(3)-C(12)-C(13)	110.1(4)
N(3)-C(12)-C(15)	124.5(4)
C(13)-C(12)-C(15)	125.4(4)
C(12)-C(13)-C(14)	108.1(4)
N(4)-C(14)-C(13)	105.7(4)
N(4)-C(14)-C(19)	131.8(4)
C(13)-C(14)-C(19)	122.4(4)
C(12)-C(15)-C(16)	109.4(4)
C(12)-C(15)-C(17)	109.5(4)
C(16)-C(15)-C(17)	108.6(4)
C(12)-C(15)-C(18)	112.0(4)
C(16)-C(15)-C(18)	107.9(4)
C(17)-C(15)-C(18)	109.4(4)

C(14)-C(19)-C(20)	106.3(4)
C(14)-C(19)-C(21)	106.9(4)
C(20)-C(19)-C(21)	108.0(4)
C(14)-C(19)-C(22)	119.0(4)
C(20)-C(19)-C(22)	107.7(4)
C(21)-C(19)-C(22)	108.5(4)
N(4)-C(23)-N(2)	112.5(3)
N(4)-C(23)-Si(1)	112.2(3)
N(2)-C(23)-Si(1)	112.4(3)
N(5)-C(26)-C(27)	123.5(4)
N(5)-C(26)-C(31)	120.6(4)
C(27)-C(26)-C(31)	115.9(4)
C(26)-C(27)-C(28)	121.3(4)
C(27)-C(28)-C(29)	121.6(4)
C(28)-C(29)-C(30)	118.0(4)
C(29)-C(30)-C(31)	120.1(4)
C(26)-C(31)-C(30)	122.9(4)
C(101)-C(102)-C(103)	112.1(13)
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_diffrn_radiation_monochromator   'graphite'
_diffrn_radiation_type            'Mo K\a'
_diffrn_radiation_wavelength           0.71073
_diffrn_measurement_method        \w

_computing_data_collection        'COLLECT (Nonius, 1997-2001).'
_computing_cell_refinement        'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_computing_data_reduction         'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
```

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_computing_structure_solution     'SIR92 (Altomare et al., 1994)'
_computing_structure_refinement   'CRYSTALS (Betteridge et al., 2003)'
_computing_publication_material   'CRYSTALS (Betteridge et al., 2003)'
_computing_molecular_graphics     'CAMERON (Watkin et al., 1996)'

_diffrn_standards_interval_time   .
_diffrn_standards_interval_count  .
_diffrn_standards_number          0
_diffrn_standards_decay_%         ?

_diffrn_ambient_temperature        150
_diffrn_reflns_number             15200
_reflns_number_total              9500
_diffrn_reflns_av_R_equivalents   0.031


_diffrn_reflns_theta_min          5.114
_diffrn_reflns_theta_max          27.476
_diffrn_measured_fraction_theta_max 0.984

_diffrn_reflns_theta_full         26.377
_diffrn_measured_fraction_theta_full 0.986


_diffrn_reflns_limit_h_min        -11
_diffrn_reflns_limit_h_max        12
_diffrn_reflns_limit_k_min        -19
_diffrn_reflns_limit_k_max        18
_diffrn_reflns_limit_l_min        -19
_diffrn_reflns_limit_l_max        19
_reflns_limit_h_min               -12
_reflns_limit_h_max               12
_reflns_limit_k_min               -19
_reflns_limit_k_max               19
_reflns_limit_l_min               0
_reflns_limit_l_max               19

_oxford_diffrn_Wilson_B_factor    3.00
_oxford_diffrn_Wilson_scale       2.76

_atom_sites_solution_primary      direct
_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens    geom

_refine_diff_density_min          -0.72
_refine_diff_density_max          1.16


# The current dictionary definitions do not cover the
# situation where the reflections used for refinement were
# selected by a user-defined sigma threshold


# The values actually used during refinement
_oxford_reflns_threshold_expression_ref     I>3.0\s(I)
_refine_ls_number_reflns          6134
_refine_ls_number_restraints      45
_refine_ls_number_parameters      482
_oxford_refine_ls_R_factor_ref    0.0723
_refine_ls_wR_factor_ref          0.0815
_refine_ls_goodness_of_fit_ref    1.1028
```

```
_refine_ls_shift/su_max           0.004605


# The values computed from all data
_oxford_reflns_number_all         9500
_refine_ls_R_factor_all           0.1082
_refine_ls_wR_factor_all          0.1119

# The values computed with a 2 sigma cutoff - a la SHELX
_reflns_threshold_expression      I>2.0\s(I)
_reflns_number_gt                 6818
_refine_ls_R_factor_gt            0.0785
_refine_ls_wR_factor_gt           0.0858

_chemical_absolute_configuration  '.'


_refine_ls_structure_factor_coef  F
_refine_ls_matrix_type            full
_refine_ls_hydrogen_treatment     mixed
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 1.70 1.39 1.34 0.250 0.256
;
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C.,
Polidori, G. & Camalli, M. (1994). J. Appl. Cryst. 27, 435.

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Crystallography Laboratory, Oxford, UK.
;

# Uequiv = arithmetic mean of Ui i.e. Ueqiv = (U1+U2+U3)/3


loop_
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_atom_site_type_symbol
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_atom_site_occupancy
_atom_site_adp_type
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
_oxford_atom_site_special_shape
_atom_site_attached_hydrogens
Ca1 Ca 0.17178(6) 0.21733(4) 0.19228(4) 0.0325 1.0000 Uani D U . . . . .
B1 B -0.0986(4) 0.1641(3) 0.1598(3) 0.0465 1.0000 Uani D . . . . . .
B2 B 0.5026(3) 0.7347(2) 0.2961(2) 0.0308 1.0000 Uani . . . . . . .
O1 O 0.2711(3) 0.1010(2) 0.11708(18) 0.0650 1.0000 Uani . U . . . . .
O2 O 0.2337(2) 0.14218(15) 0.32682(13) 0.0400 1.0000 Uani . . . . . . .
O3 O 0.1447(2) 0.35841(15) 0.26887(15) 0.0399 1.0000 Uani . . . . . . .
O4 O 0.1595(2) 0.29237(18) 0.05527(14) 0.0476 1.0000 Uani . . . . . . .
O5 O 0.41818(19) 0.27187(15) 0.23633(13) 0.0372 1.0000 Uani . . . . . . .
C1 C 0.4101(4) 0.0651(4) 0.1505(4) 0.0850 1.0000 Uani . U . . . . .
C2 C 0.3916(8) -0.0245(5) 0.1244(5) 0.1321 1.0000 Uani . U . . . . .
C3 C 0.2309(7) -0.0456(4) 0.0780(4) 0.0995 1.0000 Uani . U . . . . .
C4 C 0.1997(5) 0.0363(3) 0.0443(3) 0.0676 1.0000 Uani . U . . . . .
C5 C 0.2385(5) 0.1821(3) 0.4164(2) 0.0575 1.0000 Uani . . . . . . .
C6 C 0.1398(4) 0.1246(3) 0.4526(2) 0.0566 1.0000 Uani . . . . . . .
C7 C 0.1398(7) 0.0350(3) 0.4100(3) 0.0829 1.0000 Uani . . . . . . .
C8 C 0.2007(5) 0.0459(3) 0.3268(3) 0.0605 1.0000 Uani . . . . . . .
C9 C 0.0157(3) 0.3843(2) 0.2959(2) 0.0471 1.0000 Uani . . . . . . .
C10 C -0.0087(4) 0.4769(2) 0.2643(2) 0.0487 1.0000 Uani . . . . . . .
C11 C 0.1445(4) 0.5194(2) 0.2841(3) 0.0485 1.0000 Uani . . . . . . .
C12 C 0.2388(4) 0.4402(2) 0.2856(3) 0.0534 1.0000 Uani . . . . . . .
C13 C 0.1957(5) 0.2614(3) -0.0288(2) 0.0591 1.0000 Uani . . . . . . .
C14 C 0.1792(5) 0.3409(3) -0.0836(2) 0.0632 1.0000 Uani . . . . . . .
C15 C 0.0598(6) 0.3885(3) -0.0549(3) 0.0683 1.0000 Uani . . . . . . .
C16 C 0.0731(5) 0.3710(3) 0.0404(3) 0.0683 1.0000 Uani . . . . . . .
C17 C 0.4953(3) 0.3078(3) 0.1739(2) 0.0560 1.0000 Uani . . . . . . .
C18 C 0.6297(3) 0.3550(3) 0.2315(3) 0.0566 1.0000 Uani . . . . . . .
C19 C 0.6629(3) 0.2987(3) 0.3117(2) 0.0473 1.0000 Uani . . . . . . .
C20 C 0.5151(3) 0.2725(2) 0.3244(2) 0.0395 1.0000 Uani . . . . . . .
C21 C 0.5848(3) 0.8354(2) 0.30026(19) 0.0341 1.0000 Uani . . . . . . .
C22 C 0.5608(3) 0.9094(2) 0.3567(2) 0.0432 1.0000 Uani . . . . . . .
C23 C 0.6316(4) 0.9938(2) 0.3618(3) 0.0553 1.0000 Uani . . . . . . .
C24 C 0.7306(4) 1.0073(3) 0.3096(3) 0.0610 1.0000 Uani . . . . . . .
C25 C 0.7573(4) 0.9363(3) 0.2537(3) 0.0538 1.0000 Uani . . . . . . .
C26 C 0.6858(3) 0.8520(2) 0.2493(2) 0.0432 1.0000 Uani . . . . . . .
C27 C 0.6088(3) 0.66806(19) 0.36035(17) 0.0303 1.0000 Uani . . . . . . .
C28 C 0.7585(3) 0.6781(2) 0.37727(18) 0.0327 1.0000 Uani . . . . . . .
C29 C 0.8492(3) 0.6182(2) 0.4257(2) 0.0383 1.0000 Uani . . . . . . .
C30 C 0.7920(3) 0.5443(2) 0.4587(2) 0.0389 1.0000 Uani . . . . . . .
C31 C 0.6450(3) 0.5323(2) 0.4438(2) 0.0406 1.0000 Uani . . . . . . .
C32 C 0.5558(3) 0.5934(2) 0.39660(19) 0.0367 1.0000 Uani . . . . . . .
C33 C 0.4614(3) 0.6865(2) 0.19146(18) 0.0331 1.0000 Uani . . . . . . .
C34 C 0.4130(3) 0.7369(2) 0.1165(2) 0.0420 1.0000 Uani . . . . . . .
C35 C 0.3631(4) 0.6970(3) 0.0286(2) 0.0496 1.0000 Uani . . . . . . .
C36 C 0.3602(4) 0.6044(3) 0.0117(2) 0.0506 1.0000 Uani . . . . . . .
C37 C 0.4098(4) 0.5524(3) 0.0826(2) 0.0515 1.0000 Uani . . . . . . .
C38 C 0.4590(3) 0.5939(2) 0.1707(2) 0.0412 1.0000 Uani . . . . . . .
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C39 C 0.3544(3) 0.7494(2) 0.32983(19) 0.0329 1.0000 Uani . . . . . .
C40 C 0.3500(3) 0.7539(2) 0.4214(2) 0.0423 1.0000 Uani . . . . . .
C41 C 0.2287(4) 0.7768(3) 0.4513(2) 0.0497 1.0000 Uani . . . . . .
C42 C 0.1054(3) 0.7959(2) 0.3906(3) 0.0496 1.0000 Uani . . . . . .
C43 C 0.1040(3) 0.7915(2) 0.2999(3) 0.0481 1.0000 Uani . . . . . .
C44 C 0.2263(3) 0.7688(2) 0.2705(2) 0.0390 1.0000 Uani . . . . . .
H1 H -0.221(5) 0.1404(15) 0.1453(13) 0.075(7) 1.0000 Uiso D . . . . . .
H2 H -0.0827(11) 0.2344(17) 0.128(3) 0.075(7) 1.0000 Uiso D . . . . . .
H3 H -0.0491(16) 0.182(3) 0.2396(8) 0.075(7) 1.0000 Uiso D . . . . . .
H4 H -0.0302(14) 0.1085(15) 0.129(3) 0.075(7) 1.0000 Uiso D . . . . . .
H11 H 0.4382 0.0752 0.2145 0.0969 1.0000 Uiso R . . . . . .
H12 H 0.4811 0.0917 0.1248 0.0969 1.0000 Uiso R . . . . . .
H21 H 0.4155 -0.0582 0.1760 0.1260 1.0000 Uiso R . . . . . .
H22 H 0.4499 -0.0409 0.0840 0.1260 1.0000 Uiso R . . . . . .
H31 H 0.2181 -0.0933 0.0312 0.1116 1.0000 Uiso R . . . . . .
H32 H 0.1745 -0.0596 0.1193 0.1116 1.0000 Uiso R . . . . . .
H41 H 0.2369 0.0424 -0.0076 0.0782 1.0000 Uiso R . . . . . .
H42 H 0.0994 0.0436 0.0292 0.0782 1.0000 Uiso R . . . . . .
H51 H 0.2084 0.2424 0.4140 0.0715 1.0000 Uiso R . . . . . .
H52 H 0.3330 0.1824 0.4532 0.0715 1.0000 Uiso R . . . . . .
H61 H 0.1716 0.1248 0.5164 0.0691 1.0000 Uiso R . . . . . .
H62 H 0.0459 0.1460 0.4378 0.0691 1.0000 Uiso R . . . . . .
H71 H 0.0455 0.0076 0.3928 0.1010 1.0000 Uiso R . . . . . .
H72 H 0.1996 -0.0012 0.4503 0.1010 1.0000 Uiso R . . . . . .
H81 H 0.1311 0.0247 0.2734 0.0762 1.0000 Uiso R . . . . . .
H82 H 0.2847 0.0132 0.3303 0.0762 1.0000 Uiso R . . . . . .
H91 H 0.0290 0.3857 0.3597 0.0584 1.0000 Uiso R . . . . . .
H92 H -0.0628 0.3433 0.2675 0.0584 1.0000 Uiso R . . . . . .
H101 H -0.0658 0.5097 0.2974 0.0596 1.0000 Uiso R . . . . . .
H102 H -0.0530 0.4740 0.2015 0.0596 1.0000 Uiso R . . . . . .
H111 H 0.1557 0.5566 0.2378 0.0588 1.0000 Uiso R . . . . . .
H112 H 0.1670 0.5542 0.3408 0.0588 1.0000 Uiso R . . . . . .
H121 H 0.3033 0.4408 0.3432 0.0643 1.0000 Uiso R . . . . . .
H122 H 0.2914 0.4429 0.2402 0.0643 1.0000 Uiso R . . . . . .
H131 H 0.2912 0.2425 -0.0178 0.0748 1.0000 Uiso R . . . . . .
H132 H 0.1316 0.2126 -0.0591 0.0748 1.0000 Uiso R . . . . . .
H141 H 0.1549 0.3227 -0.1466 0.0785 1.0000 Uiso R . . . . . .
H142 H 0.2648 0.3786 -0.0694 0.0785 1.0000 Uiso R . . . . . .
H151 H 0.0690 0.4517 -0.0604 0.0866 1.0000 Uiso R . . . . . .
H152 H -0.0301 0.3647 -0.0910 0.0866 1.0000 Uiso R . . . . . .
H161 H -0.0188 0.3580 0.0511 0.0954 1.0000 Uiso R . . . . . .
H162 H 0.1184 0.4219 0.0792 0.0954 1.0000 Uiso R . . . . . .
H171 H 0.5185 0.2598 0.1360 0.0722 1.0000 Uiso R . . . . . .
H172 H 0.4391 0.3489 0.1376 0.0722 1.0000 Uiso R . . . . . .
H181 H 0.6131 0.4155 0.2499 0.0706 1.0000 Uiso R . . . . . .
H182 H 0.7051 0.3553 0.2008 0.0706 1.0000 Uiso R . . . . . .
H191 H 0.7112 0.2466 0.2983 0.0583 1.0000 Uiso R . . . . . .
H192 H 0.7196 0.3327 0.3638 0.0583 1.0000 Uiso R . . . . . .
H201 H 0.4886 0.3156 0.3658 0.0481 1.0000 Uiso R . . . . . .
H202 H 0.5142 0.2142 0.3464 0.0481 1.0000 Uiso R . . . . . .
H221 H 0.4941 0.9015 0.3931 0.0513 1.0000 Uiso R . . . . . .
H231 H 0.6123 1.0424 0.4005 0.0642 1.0000 Uiso R . . . . . .
H241 H 0.7791 1.0648 0.3125 0.0729 1.0000 Uiso R . . . . . .
H251 H 0.8244 0.9450 0.2177 0.0656 1.0000 Uiso R . . . . . .
H261 H 0.7070 0.8037 0.2110 0.0528 1.0000 Uiso R . . . . . .
H281 H 0.8000 0.7280 0.3549 0.0391 1.0000 Uiso R . . . . . .
H291 H 0.9502 0.6279 0.4363 0.0462 1.0000 Uiso R . . . . . .
H301 H 0.8526 0.5025 0.4910 0.0474 1.0000 Uiso R . . . . . .
H311 H 0.6042 0.4819 0.4660 0.0493 1.0000 Uiso R . . . . . .
H321 H 0.4551 0.5840 0.3884 0.0442 1.0000 Uiso R . . . . . .
H341 H 0.4151 0.8009 0.1264 0.0515 1.0000 Uiso R . . . . . .
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H351 H 0.3305 0.7337 -0.0197 0.0606 1.0000 Uiso R . . . . . .
H361 H 0.3242 0.5767 -0.0478 0.0593 1.0000 Uiso R . . . . . .
H371 H 0.4113 0.4887 0.0716 0.0619 1.0000 Uiso R . . . . . .
H381 H 0.4922 0.5566 0.2185 0.0505 1.0000 Uiso R . . . . . .
H401 H 0.4334 0.7405 0.4647 0.0511 1.0000 Uiso R . . . . . .
H411 H 0.2312 0.7794 0.5141 0.0618 1.0000 Uiso R . . . . . .
H421 H 0.0227 0.8122 0.4110 0.0622 1.0000 Uiso R . . . . . .
H431 H 0.0193 0.8039 0.2572 0.0579 1.0000 Uiso R . . . . . .
H441 H 0.2224 0.7662 0.2075 0.0468 1.0000 Uiso R . . . . . .
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_atom_site_aniso_U_12
Ca1 0.0243(3) 0.0445(3) 0.0273(3) -0.0007(2) 0.00450(19) 0.0003(2)
B1 0.0292(16) 0.055(2) 0.051(2) 0.0046(17) 0.0039(14) -0.0091(15)
B2 0.0240(13) 0.0385(17) 0.0289(14) 0.0019(12) 0.0044(11) 0.0025(12)
O1 0.0406(13) 0.0880(19) 0.0555(15) -0.0349(14) 0.0001(11) 0.0127(12)
O2 0.0419(11) 0.0474(12) 0.0296(10) 0.0011(9) 0.0082(8) -0.0033(9)
O3 0.0272(9) 0.0439(12) 0.0487(12) -0.0041(9) 0.0129(9) -0.0070(8)
O4 0.0387(11) 0.0755(16) 0.0324(11) 0.0129(10) 0.0115(9) 0.0189(11)
O5 0.0249(9) 0.0548(13) 0.0321(10) 0.0087(9) 0.0067(8) -0.0036(8)
C1 0.042(2) 0.107(4) 0.092(3) -0.048(3) 0.004(2) 0.021(2)
C2 0.124(5) 0.107(4) 0.128(5) -0.041(4) -0.041(4) 0.069(4)
C3 0.116(4) 0.082(4) 0.085(3) -0.017(3) 0.001(3) 0.002(3)
C4 0.059(2) 0.075(3) 0.057(2) -0.029(2) -0.0011(18) 0.000(2)
C5 0.087(3) 0.052(2) 0.0341(16) -0.0026(15) 0.0201(17) -0.0122(19)
C6 0.052(2) 0.081(3) 0.0383(17) 0.0033(17) 0.0164(15) -0.0109(18)
C7 0.130(5) 0.063(3) 0.055(2) 0.006(2) 0.022(3) -0.019(3)
C8 0.092(3) 0.043(2) 0.052(2) 0.0068(16) 0.023(2) 0.0209(19)
C9 0.0359(15) 0.053(2) 0.0547(19) -0.0099(15) 0.0214(14) -0.0059(14)
C10 0.0413(16) 0.055(2) 0.0495(18) -0.0094(15) 0.0135(14) 0.0082(15)
C11 0.0473(18) 0.0448(19) 0.0530(19) 0.0004(15) 0.0125(15) -0.0006(14)
C12 0.0361(16) 0.0434(19) 0.079(2) -0.0054(17) 0.0144(16) -0.0109(14)
C13 0.065(2) 0.080(3) 0.0346(17) 0.0033(17) 0.0145(16) 0.021(2)
C14 0.090(3) 0.066(2) 0.0375(18) 0.0005(16) 0.0260(19) -0.001(2)
C15 0.093(3) 0.068(3) 0.048(2) 0.0150(19) 0.018(2) 0.028(2)
C16 0.070(3) 0.091(3) 0.058(2) 0.030(2) 0.031(2) 0.037(2)
C17 0.0324(15) 0.096(3) 0.0439(18) 0.0292(19) 0.0106(13) -0.0039(17)
C18 0.0315(15) 0.073(3) 0.066(2) 0.032(2) 0.0071(15) -0.0045(16)
C19 0.0289(14) 0.060(2) 0.0518(19) 0.0153(16) 0.0038(13) -0.0010(14)
C20 0.0307(13) 0.0513(18) 0.0347(14) 0.0075(13) 0.0034(11) -0.0029(12)
C21 0.0239(12) 0.0395(15) 0.0355(14) 0.0080(12) -0.0014(10) 0.0024(11)
C22 0.0409(16) 0.0413(17) 0.0432(17) 0.0077(13) -0.0005(13) 0.0051(13)
C23 0.053(2) 0.0349(17) 0.070(2) 0.0072(16) -0.0028(17) 0.0044(15)
C24 0.049(2) 0.0389(19) 0.087(3) 0.0242(19) -0.0040(19) -0.0041(15)
C25 0.0355(16) 0.054(2) 0.071(2) 0.0273(19) 0.0050(16) -0.0031(15)
C26 0.0310(14) 0.0481(18) 0.0514(18) 0.0138(14) 0.0086(13) 0.0019(13)
C27 0.0278(12) 0.0366(15) 0.0242(12) -0.0030(10) 0.0039(10) -0.0007(11)
C28 0.0286(13) 0.0354(15) 0.0334(14) 0.0001(11) 0.0075(11) -0.0011(11)
C29 0.0287(13) 0.0475(17) 0.0369(15) 0.0010(13) 0.0043(11) 0.0060(12)
C30 0.0414(15) 0.0430(17) 0.0319(14) 0.0062(12) 0.0053(12) 0.0130(13)
C31 0.0431(16) 0.0448(17) 0.0356(15) 0.0099(13) 0.0109(13) 0.0012(13)
C32 0.0292(13) 0.0473(17) 0.0323(14) 0.0045(12) 0.0053(11) -0.0025(12)
C33 0.0245(12) 0.0468(17) 0.0283(13) 0.0023(11) 0.0072(10) 0.0003(11)
C34 0.0415(16) 0.0533(19) 0.0307(14) 0.0051(13) 0.0065(12) 0.0048(14)
C35 0.0423(17) 0.079(3) 0.0282(14) 0.0107(15) 0.0071(13) 0.0063(16)
C36 0.0489(18) 0.071(2) 0.0300(15) -0.0087(15) 0.0108(13) 0.0007(16)
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C38 0.0443(16) 0.0485(18) 0.0313(14) 0.0010(13) 0.0106(12) 0.0011(14)
C39 0.0258(12) 0.0371(15) 0.0342(14) -0.0008(11) 0.0057(10) -0.0022(11)
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C41 0.0490(18) 0.060(2) 0.0458(18) 0.0006(15) 0.0243(15) 0.0030(16)
C42 0.0344(15) 0.051(2) 0.068(2) -0.0046(16) 0.0248(15) 0.0004(14)
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_exptl_crystal_density_method       'not measured'
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_exptl_crystal_F_000             1036
_exptl_absorpt_coefficient_mu    0.168

_exptl_absorpt_correction_type   multi-scan
_exptl_absorpt_process_details   'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_exptl_absorpt_correction_T_min  0.98
_exptl_absorpt_correction_T_max  0.98
_diffrn_measurement_device       'Nonius KappaCCD'
_diffrn_measurement_device_type  'Area'
_diffrn_radiation_monochromator  'graphite'
_diffrn_radiation_type           'Mo K\a'
_diffrn_radiation_wavelength          0.71073
_diffrn_measurement_method       \w

_computing_data_collection       'COLLECT (Nonius, 1997-2001).'
_computing_cell_refinement       'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_computing_data_reduction        'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_computing_structure_solution    'SIR92 (Altomare et al., 1994)'
_computing_structure_refinement  'CRYSTALS (Betteridge et al., 2003)'
_computing_publication_material  'CRYSTALS (Betteridge et al., 2003)'
_computing_molecular_graphics    'CAMERON (Watkin et al., 1996)'

_diffrn_standards_interval_time  .
_diffrn_standards_interval_count .
_diffrn_standards_number         0
_diffrn_standards_decay_%        ?

_diffrn_ambient_temperature       150
_diffrn_reflns_number            15844
_reflns_number_total             9271
_diffrn_reflns_av_R_equivalents  0.019


_diffrn_reflns_theta_min         5.172
_diffrn_reflns_theta_max         25.032
_diffrn_measured_fraction_theta_max 0.984

_diffrn_reflns_theta_full        25.032
_diffrn_measured_fraction_theta_full 0.984


_diffrn_reflns_limit_h_min       -12
_diffrn_reflns_limit_h_max       12
_diffrn_reflns_limit_k_min       -17
_diffrn_reflns_limit_k_max       17
_diffrn_reflns_limit_l_min       -20
_diffrn_reflns_limit_l_max       20
_reflns_limit_h_min              -12
_reflns_limit_h_max              12
_reflns_limit_k_min              -17
_reflns_limit_k_max              17
_reflns_limit_l_min              0
_reflns_limit_l_max              20

_oxford_diffrn_Wilson_B_factor   2.35
_oxford_diffrn_Wilson_scale      0.62

_atom_sites_solution_primary     direct
_atom_sites_solution_secondary   difmap
_atom_sites_solution_hydrogens   geom
```

```
_refine_diff_density_min         -0.37
_refine_diff_density_max         0.92


# The current dictionary definitions do not cover the
# situation where the reflections used for refinement were
# selected by a user-defined sigma threshold


# The values actually used during refinement
_oxford_reflns_threshold_expression_ref     I>3.0\s(I)
_refine_ls_number_reflns         7488
_refine_ls_number_restraints     38
_refine_ls_number_parameters     647
_oxford_refine_ls_R_factor_ref   0.0440
_refine_ls_wR_factor_ref         0.0464
_refine_ls_goodness_of_fit_ref   1.0955
_refine_ls_shift/su_max          0.019404


# The values computed from all data
_oxford_reflns_number_all        9271
_refine_ls_R_factor_all          0.0553
_refine_ls_wR_factor_all         0.0594

# The values computed with a 2 sigma cutoff - a la SHELX
_reflns_threshold_expression     I>2.0\s(I)
_reflns_number_gt                7647
_refine_ls_R_factor_gt           0.0450
_refine_ls_wR_factor_gt          0.0471

_chemical_absolute_configuration  '.'


_refine_ls_structure_factor_coef  F
_refine_ls_matrix_type           full
_refine_ls_hydrogen_treatment    mixed
_refine_ls_weighting_scheme      calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 0.409 0.325 0.243 0.983E-01 0.606E-01
;
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C.,
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Crystallography Laboratory, Oxford, UK.
;

Uequiv = arithmetic mean of Ui i.e. Ueqiv = (U1+U2+U3)/3

loop_
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_adp_type
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
_oxford_atom_site_special_shape
_atom_site_attached_hydrogens
Ca1 Ca 0.80347(3) 0.79001(2) 0.179761(19) 0.0231 1.0000 Uani . . . . . .
B1 B 1.0242(2) 0.76821(17) 0.09156(14) 0.0361 1.0000 Uani . . . . . .
B2 B 1.14384(19) 1.15109(13) 0.29485(11) 0.0246 1.0000 Uani . . . . . .
N1 N 0.79079(14) 0.63698(10) 0.25332(8) 0.0264 1.0000 Uani . . . . . .
N2 N 0.67919(14) 0.59845(10) 0.25601(8) 0.0254 1.0000 Uani . . . . . .
N3 N 0.65692(14) 0.71660(10) 0.11401(8) 0.0254 1.0000 Uani . . . . . .
N4 N 0.55331(14) 0.68156(10) 0.15801(8) 0.0252 1.0000 Uani . . . . . .
N5 N 0.58380(14) 0.80467(10) 0.26392(8) 0.0257 1.0000 Uani . . . . . .
N6 N 0.52425(14) 0.72910(10) 0.28511(8) 0.0264 1.0000 Uani . . . . . .
O1 O 0.72064(12) 0.93903(8) 0.13062(8) 0.0325 1.0000 Uani . . . . . .
O2 O 0.86991(12) 0.83025(9) 0.29346(7) 0.0299 1.0000 Uani . . . . . .
O3 O 1.68470(17) 1.37703(14) 0.08949(13) 0.0702 1.0000 Uani . . . . . .
O4 O 0.4129(2) 0.42062(16) 0.46103(14) 0.0818 1.0000 Uani . U . . . .
C1 C 0.88288(18) 0.56775(12) 0.27214(10) 0.0295 1.0000 Uani . . . . . .
C2 C 0.83135(19) 0.48594(13) 0.28609(11) 0.0333 1.0000 Uani . . . . . .
C3 C 0.70084(19) 0.50722(12) 0.27511(10) 0.0294 1.0000 Uani . . . . . .
C4 C 1.01991(19) 0.58319(14) 0.27673(13) 0.0400 1.0000 Uani . . . . . .
C5 C 0.5966(2) 0.44945(13) 0.28053(13) 0.0398 1.0000 Uani . . . . . .
C6 C 0.62640(18) 0.72821(12) 0.04149(10) 0.0273 1.0000 Uani . . . . . .
C7 C 0.50325(19) 0.70211(13) 0.03929(11) 0.0319 1.0000 Uani . . . . . .
C8 C 0.45854(17) 0.67275(12) 0.11409(11) 0.0291 1.0000 Uani . . . . . .
C9 C 0.7195(2) 0.76287(14) -0.02402(11) 0.0339 1.0000 Uani . . . . . .
C10 C 0.33475(19) 0.63788(15) 0.14858(13) 0.0403 1.0000 Uani . . . . . .
C11 C 0.52956(17) 0.86065(13) 0.31670(10) 0.0298 1.0000 Uani . . . . . .
C12 C 0.43795(19) 0.82038(14) 0.37131(11) 0.0352 1.0000 Uani . . . . . .
C13 C 0.43575(18) 0.73666(13) 0.35015(10) 0.0322 1.0000 Uani . . . . . .
C14 C 0.5644(2) 0.95306(13) 0.31186(12) 0.0362 1.0000 Uani . . . . . .
C15 C 0.3588(2) 0.66307(15) 0.38525(13) 0.0444 1.0000 Uani . . . . . .
C16 C 0.55649(17) 0.65352(12) 0.23987(10) 0.0253 1.0000 Uani . . . . . .

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C17 C 0.7927(2) 1.01456(14) 0.11624(14) 0.0443 1.0000 Uani . . . . . .
C18 C 0.6907(3) 1.09692(15) 0.11398(15) 0.0536 1.0000 Uani . . . . . .
C19 C 0.5743(2) 1.06717(15) 0.08713(13) 0.0455 1.0000 Uani . . . . . .
C20 C 0.6076(2) 0.96614(14) 0.08958(14) 0.0422 1.0000 Uani . . . . . .
C21 C 0.84388(19) 0.78707(14) 0.37222(10) 0.0343 1.0000 Uani . . . . . .
C22 C 0.9680(2) 0.78444(16) 0.41057(12) 0.0436 1.0000 Uani . . . . . .
C23 C 1.0639(2) 0.82516(14) 0.34639(13) 0.0395 1.0000 Uani . . . . . .
C24 C 0.97296(19) 0.88413(13) 0.29447(12) 0.0345 1.0000 Uani . . . . . .
C25 C 0.98666(18) 1.18519(12) 0.32161(10) 0.0273 1.0000 Uani . . . . . .
C26 C 0.9535(2) 1.24615(13) 0.37781(11) 0.0350 1.0000 Uani . . . . . .
C27 C 0.8242(2) 1.27183(15) 0.40947(13) 0.0483 1.0000 Uani . . . . . .
C28 C 0.7226(2) 1.23728(17) 0.38627(14) 0.0514 1.0000 Uani . . . . . .
C29 C 0.7512(2) 1.17863(16) 0.33027(14) 0.0464 1.0000 Uani . . . . . .
C30 C 0.88112(18) 1.15347(14) 0.29872(11) 0.0347 1.0000 Uani . . . . . .
C31 C 1.16616(16) 1.07758(12) 0.23089(10) 0.0249 1.0000 Uani . . . . . .
C32 C 1.11265(18) 1.09913(13) 0.16035(10) 0.0310 1.0000 Uani . . . . . .
C33 C 1.1328(2) 1.03974(15) 0.10390(11) 0.0374 1.0000 Uani . . . . . .
C34 C 1.2097(2) 0.95590(15) 0.11559(12) 0.0393 1.0000 Uani . . . . . .
C35 C 1.2669(2) 0.93303(14) 0.18347(12) 0.0359 1.0000 Uani . . . . . .
C36 C 1.24459(17) 0.99297(12) 0.23986(11) 0.0283 1.0000 Uani . . . . . .
C37 C 1.20222(17) 1.10302(12) 0.37578(10) 0.0251 1.0000 Uani . . . . . .
C38 C 1.14413(18) 1.03111(12) 0.41821(10) 0.0284 1.0000 Uani . . . . . .
C39 C 1.18789(19) 0.98412(13) 0.48577(10) 0.0314 1.0000 Uani . . . . . .
C40 C 1.29302(19) 1.00865(13) 0.51440(11) 0.0334 1.0000 Uani . . . . . .
C41 C 1.35038(19) 1.08113(14) 0.47601(11) 0.0333 1.0000 Uani . . . . . .
C42 C 1.30511(18) 1.12734(13) 0.40806(10) 0.0284 1.0000 Uani . . . . . .
C43 C 1.22029(17) 1.23461(12) 0.25198(10) 0.0253 1.0000 Uani . . . . . .
C44 C 1.15642(19) 1.31985(12) 0.22484(11) 0.0303 1.0000 Uani . . . . . .
C45 C 1.2242(2) 1.38661(13) 0.18266(11) 0.0352 1.0000 Uani . . . . . .
C46 C 1.3596(2) 1.37107(13) 0.16702(11) 0.0349 1.0000 Uani . . . . . .
C47 C 1.42646(19) 1.28787(13) 0.19320(11) 0.0330 1.0000 Uani . . . . . .
C48 C 1.35773(18) 1.22148(12) 0.23362(10) 0.0281 1.0000 Uani . . . . . .
C49 C 1.6883(2) 1.46413(19) 0.05091(16) 0.0602 1.0000 Uani D . . . . . .
C50 C 1.8133(5) 1.4942(3) 0.0624(5) 0.0473 0.3000 Uani D . . . . . .
C51 C 1.9013(2) 1.40637(18) 0.07893(16) 0.0592 1.0000 Uani D . . . . . .
C52 C 1.8110(2) 1.33967(16) 0.10982(15) 0.0526 1.0000 Uani D . . . . . .
C53 C 0.3251(2) 0.4498(2) 0.52472(14) 0.0577 1.0000 Uani D U . . . . .
C54 C 0.1907(3) 0.4659(2) 0.50089(17) 0.0659 1.0000 Uani D U . . . . .
C55 C 0.2075(4) 0.3993(3) 0.4405(2) 0.1127 1.0000 Uani D U . . . . .
C56 C 0.3488(4) 0.3589(3) 0.4380(3) 0.1083 1.0000 Uani D U . . . . .
C501 C 1.8289(3) 1.4686(3) 0.0216(2) 0.0579 0.7000 Uani D . . . . . .
H1 H 1.123(2) 0.7614(17) 0.0530(15) 0.055(7) 1.0000 Uiso . . . . . .
H2 H 0.948(3) 0.8341(19) 0.0704(16) 0.064(8) 1.0000 Uiso . . . . . .
H3 H 1.039(3) 0.7801(18) 0.1556(16) 0.063(8) 1.0000 Uiso . . . . . .
H4 H 0.966(2) 0.7097(16) 0.0989(13) 0.046(6) 1.0000 Uiso . . . . . .
H21 H 0.8775 0.4277 0.3003 0.0399 1.0000 Uiso R . . . . . .
H41 H 1.0723 0.5271 0.2905 0.0493 1.0000 Uiso R . . . . . .
H42 H 1.0185 0.6226 0.3149 0.0493 1.0000 Uiso R . . . . . .
H43 H 1.0558 0.6096 0.2278 0.0493 1.0000 Uiso R . . . . . .
H51 H 0.5646 0.4548 0.2317 0.0497 1.0000 Uiso R . . . . . .
H52 H 0.5266 0.4683 0.3187 0.0497 1.0000 Uiso R . . . . . .
H53 H 0.6320 0.3883 0.2946 0.0497 1.0000 Uiso R . . . . . .
H71 H 0.4600 0.7042 -0.0054 0.0406 1.0000 Uiso R . . . . . .
H91 H 0.7988 0.7695 -0.0059 0.0439 1.0000 Uiso R . . . . . .
H92 H 0.6789 0.8195 -0.0464 0.0439 1.0000 Uiso R . . . . . .
H93 H 0.7367 0.7211 -0.0616 0.0439 1.0000 Uiso R . . . . . .
H101 H 0.3553 0.5785 0.1737 0.0515 1.0000 Uiso R . . . . . .
H102 H 0.2818 0.6368 0.1088 0.0515 1.0000 Uiso R . . . . . .
H103 H 0.2883 0.6762 0.1854 0.0515 1.0000 Uiso R . . . . . .
H121 H 0.3874 0.8463 0.4146 0.0424 1.0000 Uiso R . . . . . .
H141 H 0.5163 0.9828 0.3539 0.0463 1.0000 Uiso R . . . . . .
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H142 H 0.5435 0.9865 0.2641 0.0463 1.0000 Uiso R . . . . . .
H143 H 0.6557 0.9488 0.3146 0.0463 1.0000 Uiso R . . . . . .
H151 H 0.4173 0.6102 0.4000 0.0531 1.0000 Uiso R . . . . . .
H152 H 0.3029 0.6818 0.4298 0.0531 1.0000 Uiso R . . . . . .
H153 H 0.3074 0.6504 0.3484 0.0531 1.0000 Uiso R . . . . . .
H161 H 0.4898 0.6166 0.2556 0.0314 1.0000 Uiso R . . . . . .
H171 H 0.8469 1.0131 0.0679 0.0569 1.0000 Uiso R . . . . . .
H172 H 0.8454 1.0136 0.1565 0.0569 1.0000 Uiso R . . . . . .
H181 H 0.7209 1.1448 0.0788 0.0677 1.0000 Uiso R . . . . . .
H182 H 0.6677 1.1161 0.1643 0.0677 1.0000 Uiso R . . . . . .
H191 H 0.5628 1.0942 0.0359 0.0549 1.0000 Uiso R . . . . . .
H192 H 0.4965 1.0830 0.1210 0.0549 1.0000 Uiso R . . . . . .
H201 H 0.6277 0.9497 0.0382 0.0533 1.0000 Uiso R . . . . . .
H202 H 0.5359 0.9380 0.1156 0.0533 1.0000 Uiso R . . . . . .
H211 H 0.7707 0.8208 0.3996 0.0424 1.0000 Uiso R . . . . . .
H212 H 0.8267 0.7274 0.3713 0.0424 1.0000 Uiso R . . . . . .
H221 H 0.9499 0.8199 0.4529 0.0539 1.0000 Uiso R . . . . . .
H222 H 1.0023 0.7242 0.4285 0.0539 1.0000 Uiso R . . . . . .
H231 H 1.1173 0.8596 0.3666 0.0502 1.0000 Uiso R . . . . . .
H232 H 1.1183 0.7793 0.3195 0.0502 1.0000 Uiso R . . . . . .
H241 H 0.9383 0.9393 0.3154 0.0460 1.0000 Uiso R . . . . . .
H242 H 1.0166 0.8967 0.2437 0.0460 1.0000 Uiso R . . . . . .
H261 H 1.0216 1.2709 0.3945 0.0416 1.0000 Uiso R . . . . . .
H271 H 0.8059 1.3131 0.4474 0.0545 1.0000 Uiso R . . . . . .
H281 H 0.6346 1.2540 0.4085 0.0545 1.0000 Uiso R . . . . . .
H291 H 0.6822 1.1554 0.3131 0.0546 1.0000 Uiso R . . . . . .
H301 H 0.8985 1.1129 0.2602 0.0414 1.0000 Uiso R . . . . . .
H321 H 1.0605 1.1564 0.1509 0.0392 1.0000 Uiso R . . . . . .
H331 H 1.0938 1.0566 0.0572 0.0482 1.0000 Uiso R . . . . . .
H341 H 1.2233 0.9151 0.0774 0.0492 1.0000 Uiso R . . . . . .
H351 H 1.3209 0.8763 0.1919 0.0445 1.0000 Uiso R . . . . . .
H361 H 1.2845 0.9757 0.2862 0.0357 1.0000 Uiso R . . . . . .
H381 H 1.0715 1.0137 0.3997 0.0356 1.0000 Uiso R . . . . . .
H391 H 1.1458 0.9355 0.5121 0.0383 1.0000 Uiso R . . . . . .
H401 H 1.3249 0.9760 0.5598 0.0405 1.0000 Uiso R . . . . . .
H411 H 1.4210 1.0994 0.4959 0.0412 1.0000 Uiso R . . . . . .
H421 H 1.3457 1.1771 0.3829 0.0355 1.0000 Uiso R . . . . . .
H441 H 1.0636 1.3327 0.2357 0.0372 1.0000 Uiso R . . . . . .
H451 H 1.1769 1.4430 0.1644 0.0426 1.0000 Uiso R . . . . . .
H461 H 1.4057 1.4169 0.1390 0.0441 1.0000 Uiso R . . . . . .
H471 H 1.5195 1.2763 0.1832 0.0412 1.0000 Uiso R . . . . . .
H481 H 1.4056 1.1645 0.2498 0.0346 1.0000 Uiso R . . . . . .
H491 H 1.6561 1.5082 0.0857 0.0720 1.0000 Uiso R . . . . . .
H492 H 1.6365 1.4736 0.0092 0.0720 1.0000 Uiso R . . . . . .
H501 H 1.8012 1.5302 0.1041 0.0611 0.3000 Uiso R . . . . . .
H502 H 1.8478 1.5273 0.0162 0.0611 0.3000 Uiso R . . . . . .
H511 H 1.9174 1.4382 0.1191 0.0722 1.0000 Uiso R . . . . . .
H512 H 1.9823 1.3775 0.0551 0.0722 1.0000 Uiso R . . . . . .
H521 H 1.8079 1.3283 0.1647 0.0644 1.0000 Uiso R . . . . . .
H522 H 1.8405 1.2847 0.0875 0.0644 1.0000 Uiso R . . . . . .
H531 H 0.3297 0.4046 0.5679 0.0701 1.0000 Uiso R . . . . . .
H532 H 0.3464 0.5040 0.5383 0.0701 1.0000 Uiso R . . . . . .
H541 H 0.1262 0.4521 0.5429 0.0798 1.0000 Uiso R . . . . . .
H542 H 0.1683 0.5265 0.4788 0.0798 1.0000 Uiso R . . . . . .
H551 H 0.1521 0.3544 0.4560 0.1453 1.0000 Uiso R . . . . . .
H552 H 0.1890 0.4299 0.3914 0.1453 1.0000 Uiso R . . . . . .
H561 H 0.3839 0.3473 0.3866 0.1308 1.0000 Uiso R . . . . . .
H562 H 0.3579 0.3042 0.4717 0.1308 1.0000 Uiso R . . . . . .
H5011 H 1.8478 1.5284 0.0191 0.0733 0.7000 Uiso R . . . . . .
H5012 H 1.8502 1.4484 -0.0284 0.0733 0.7000 Uiso R . . . . . .
loop_
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_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_23
_atom_site_aniso_U_13
_atom_site_aniso_U_12
Ca1 0.02238(18) 0.02458(18) 0.02264(18) -0.00379(13) -0.00331(13) -0.00296(13)
B1 0.0297(11) 0.0434(13) 0.0334(12) -0.0076(10) 0.0019(9) -0.0024(10)
B2 0.0247(10) 0.0263(10) 0.0224(9) -0.0021(8) -0.0033(7) -0.0030(8)
N1 0.0250(7) 0.0259(8) 0.0278(8) -0.0026(6) -0.0032(6) -0.0024(6)
N2 0.0271(7) 0.0237(7) 0.0246(7) -0.0007(6) -0.0022(6) -0.0037(6)
N3 0.0257(7) 0.0289(8) 0.0225(7) -0.0034(6) -0.0014(6) -0.0072(6)
N4 0.0243(7) 0.0277(8) 0.0246(7) -0.0023(6) -0.0033(6) -0.0066(6)
N5 0.0248(7) 0.0263(8) 0.0259(7) -0.0058(6) -0.0026(6) -0.0016(6)
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O2 . C24 . 1.452(2)    yes
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O3 . C52 . 1.414(3)    yes
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O4 . C56 . 1.363(4) yes
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C2 . C3 . 1.376(3) yes
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C3 . C5 . 1.486(3) yes
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C6 . C9 . 1.492(3) yes
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C11 . C14 . 1.487(3) yes
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C30 . H301 . 0.950    no
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C34 . H341 . 0.950    no
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C36 . H361 . 0.949    no
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C41 . C42 . 1.396(3)    yes
C41 . H411 . 0.949    no
C42 . H421 . 0.950    no
C43 . C44 . 1.401(3)    yes
C43 . C48 . 1.407(3)    yes
C44 . C45 . 1.397(3)    yes
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C48 . H481 . 0.949    no
C49 . C50 . 1.492(4)    yes
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C50 . H5011 . 0.923    no
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H3 . B1 . H4 . 105.7(18)    no
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C25 . B2 . C43 . 112.22(14)    yes
C31 . B2 . C43 . 104.91(13)    yes
C37 . B2 . C43 . 113.05(14)    yes
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N2 . N1 . C1 . 104.46(14)    yes
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N4 . C16 . H161 . 106.8 no
N6 . C16 . H161 . 106.6 no
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C17 . C18 . H182 . 110.3 no
C19 . C18 . H182 . 110.4 no
H181 . C18 . H182 . 109.5 no
C18 . C19 . C20 . 105.05(17) yes
C18 . C19 . H191 . 110.3 no
C20 . C19 . H191 . 110.8 no
C18 . C19 . H192 . 110.7 no
C20 . C19 . H192 . 110.3 no
H191 . C19 . H192 . 109.6 no
C19 . C20 . O1 . 107.08(17) yes
C19 . C20 . H201 . 109.8 no
O1 . C20 . H201 . 109.8 no
C19 . C20 . H202 . 110.4 no
O1 . C20 . H202 . 110.2 no
H201 . C20 . H202 . 109.5 no
O2 . C21 . C22 . 106.26(16) yes
O2 . C21 . H211 . 110.5 no
C22 . C21 . H211 . 110.4 no
O2 . C21 . H212 . 110.1 no
C22 . C21 . H212 . 110.1 no
H211 . C21 . H212 . 109.5 no

C21 . C22 . C23 . 104.48(16) yes
C21 . C22 . H221 . 110.5 no
C23 . C22 . H221 . 110.5 no
C21 . C22 . H222 . 110.9 no
C23 . C22 . H222 . 111.0 no
H221 . C22 . H222 . 109.5 no
C22 . C23 . C24 . 102.31(16) yes
C22 . C23 . H231 . 111.4 no
C24 . C23 . H231 . 111.4 no
C22 . C23 . H232 . 111.1 no
C24 . C23 . H232 . 111.0 no
H231 . C23 . H232 . 109.5 no
C23 . C24 . O2 . 103.49(15) yes
C23 . C24 . H241 . 110.7 no
O2 . C24 . H241 . 110.9 no
C23 . C24 . H242 . 111.2 no
O2 . C24 . H242 . 110.9 no
H241 . C24 . H242 . 109.5 no
B2 . C25 . C26 . 118.21(16) yes
B2 . C25 . C30 . 126.14(16) yes
C26 . C25 . C30 . 115.41(17) yes
C25 . C26 . C27 . 122.3(2) yes
C25 . C26 . H261 . 118.8 no
C27 . C26 . H261 . 118.9 no
C26 . C27 . C28 . 120.5(2) yes
C26 . C27 . H271 . 119.7 no
C28 . C27 . H271 . 119.8 no
C27 . C28 . C29 . 118.84(19) yes
C27 . C28 . H281 . 120.4 no
C29 . C28 . H281 . 120.8 no
C28 . C29 . C30 . 120.3(2) yes
C28 . C29 . H291 . 119.7 no
C30 . C29 . H291 . 120.0 no
C29 . C30 . C25 . 122.7(2) yes
C29 . C30 . H301 . 118.8 no
C25 . C30 . H301 . 118.5 no
B2 . C31 . C32 . 121.01(16) yes
B2 . C31 . C36 . 123.63(15) yes
C32 . C31 . C36 . 115.25(16) yes
C31 . C32 . C33 . 122.59(19) yes
C31 . C32 . H321 . 118.5 no
C33 . C32 . H321 . 118.9 no
C32 . C33 . C34 . 120.32(19) yes
C32 . C33 . H331 . 119.9 no
C34 . C33 . H331 . 119.7 no
C33 . C34 . C35 . 118.87(18) yes
C33 . C34 . H341 . 120.6 no
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C34 . C35 . C36 . 120.10(19) yes
C34 . C35 . H351 . 119.8 no
C36 . C35 . H351 . 120.1 no
C31 . C36 . C35 . 122.84(18) yes
C31 . C36 . H361 . 118.5 no
C35 . C36 . H361 . 118.6 no
B2 . C37 . C38 . 118.47(15) yes
B2 . C37 . C42 . 126.31(16) yes
C38 . C37 . C42 . 115.22(16) yes
C37 . C38 . C39 . 123.25(17) yes
C37 . C38 . H381 . 118.4 no
C39 . C38 . H381 . 118.4 no
C38 . C39 . C40 . 119.58(18) yes

C38 . C39 . H391 . 120.1 no
C40 . C39 . H391 . 120.3 no
C39 . C40 . C41 . 119.17(17) yes
C39 . C40 . H401 . 120.2 no
C41 . C40 . H401 . 120.6 no
C40 . C41 . C42 . 120.33(17) yes
C40 . C41 . H411 . 119.8 no
C42 . C41 . H411 . 119.9 no
C37 . C42 . C41 . 122.37(18) yes
C37 . C42 . H421 . 118.8 no
C41 . C42 . H421 . 118.8 no
B2 . C43 . C44 . 124.09(16) yes
B2 . C43 . C48 . 120.73(15) yes
C44 . C43 . C48 . 114.94(16) yes
C43 . C44 . C45 . 122.46(18) yes
C43 . C44 . H441 . 118.7 no
C45 . C44 . H441 . 118.9 no
C44 . C45 . C46 . 120.53(18) yes
C44 . C45 . H451 . 119.7 no
C46 . C45 . H451 . 119.8 no
C45 . C46 . C47 . 118.81(18) yes
C45 . C46 . H461 . 120.4 no
C47 . C46 . H461 . 120.7 no
C46 . C47 . C48 . 120.09(18) yes
C46 . C47 . H471 . 119.8 no
C48 . C47 . H471 . 120.1 no
C43 . C48 . C47 . 123.15(17) yes
C43 . C48 . H481 . 118.3 no
C47 . C48 . H481 . 118.5 no
O3 . C49 . C50 . 108.7(3) yes
O3 . C49 . C501 . 106.0(2) yes
C50 . C49 . C501 . 32.7(3) yes
O3 . C49 . H491 . 110.4 no
C50 . C49 . H491 . 79.3 no
C501 . C49 . H491 . 110.3 no
O3 . C49 . H492 . 109.9 no
C50 . C49 . H492 . 133.7 no
C501 . C49 . H492 . 110.7 no
H491 . C49 . H492 . 109.5 no
C49 . C50 . C51 . 102.7(3) yes
C49 . C50 . C501 . 73.5(4) yes
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C49 . C50 . H501 . 111.7 no
C51 . C50 . H501 . 112.0 no
C501 . C50 . H501 . 171.6 no
C49 . C50 . H502 . 110.4 no
C51 . C50 . H502 . 110.4 no
C501 . C50 . H502 . 62.1 no
H501 . C50 . H502 . 109.5 no
C49 . C50 . H5011 . 112.6 no
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C501 . C50 . H5011 . 65.0 no
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H502 . C50 . H5011 . 3.0 no
C50 . C51 . C52 . 105.1(3) yes
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C52 . C51 . C501 . 103.8(2) yes
C50 . C51 . H511 . 79.8 no
C52 . C51 . H511 . 110.8 no
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C50 . C51 . H512 . 135.4 no

C52 . C51 . H512 . 111.1 no
C501 . C51 . H512 . 111.1 no
H511 . C51 . H512 . 109.6 no
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O3 . C52 . H521 . 109.8 no
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O3 . C52 . H522 . 109.8 no
H521 . C52 . H522 . 109.5 no
O4 . C53 . C54 . 107.4(2) yes
O4 . C53 . H531 . 110.1 no
C54 . C53 . H531 . 109.7 no
O4 . C53 . H532 . 109.9 no
C54 . C53 . H532 . 110.2 no
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C53 . C54 . C55 . 100.4(2) yes
C53 . C54 . H541 . 112.1 no
C55 . C54 . H541 . 111.6 no
C53 . C54 . H542 . 111.4 no
C55 . C54 . H542 . 111.8 no
H541 . C54 . H542 . 109.5 no
C54 . C55 . C56 . 103.5(3) yes
C54 . C55 . H551 . 111.0 no
C56 . C55 . H551 . 111.2 no
C54 . C55 . H552 . 110.9 no
C56 . C55 . H552 . 110.7 no
H551 . C55 . H552 . 109.5 no
C55 . C56 . O4 . 107.0(3) yes
C55 . C56 . H561 . 110.3 no
O4 . C56 . H561 . 109.4 no
C55 . C56 . H562 . 110.0 no
O4 . C56 . H562 . 110.6 no
H561 . C56 . H562 . 109.5 no
C49 . C501 . C51 . 103.8(2) yes
C49 . C501 . C50 . 73.8(4) yes
C51 . C501 . C50 . 75.0(4) yes
C49 . C501 . H502 . 112.0 no
C51 . C501 . H502 . 113.7 no
C50 . C501 . H502 . 64.8 no
C49 . C501 . H5011 . 111.0 no
C51 . C501 . H5011 . 111.4 no
C50 . C501 . H5011 . 61.7 no
H502 . C501 . H5011 . 3.2 no
C49 . C501 . H5012 . 110.7 no
C51 . C501 . H5012 . 110.4 no
C50 . C501 . H5012 . 171.1 no
H502 . C501 . H5012 . 106.4 no
H5011 . C501 . H5012 . 109.4 no
B1 . H2 . Ca1 . 86.3(14) no
B1 . H3 . Ca1 . 84.5(14) no
B1 . H4 . Ca1 . 89.2(13) no
C50 . H502 . C501 . 53.1 no
C501 . H5011 . C50 . 53.3 no

Table 1. Crystal data and structure refinement for MGC50.

Empirical formula	C32 H44 Ca1 N12, 2(C24 H20 B1), 2(C1 H2 CL2)
Formula weight	1445.19
Crystal description	colourless block

Crystal size	0.50 x 0.50 x 0.40 mm
Temperature	150 K
Crystal system	Monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 17.3586(2) A alpha = 90 deg. b = 11.6324(2) A beta = 101.4676(6) deg. c = 19.3012(3) A gamma = 90 deg.
Reflections for cell refinement	8726
Range in theta	5 to 27 deg.
Volume, Z	3819.54(10) A^3, 2
Density (calculated)	1.257 Mg/m^3
Absorption coefficient	0.275 mm^-1
F(000)	1524
Diffractometer type	Area
Wavelength	0.71073 A
Scan type	\w
Theta range for data collection	5.104 to 27.500 deg.
Index ranges	-22<=h<=22, 0<=k<=15, 0<=l<=25
Reflections collected	16823
Independent reflections	8634 [R(merge) = 0.032]
Observed reflections	5857 [I>3sigma(I)]
Absorption correction	Semi-empirical from equivalents (Tmin = 0.87, Tmax = 0.90)
Structure solution by	direct and Fourier difference maps
Hydrogen atom location	UPDATE THIS FIELD
Hydrogen atom treatment	UPDATE THIS FIELD
Refinement method	Full-matrix least-squares on F
Weighting scheme	UPDATE THIS FIELD
Data / restraints / parameters	5316 / 0/ 457
Goodness-of-fit on F	1.1245
Final R indices [I>3sigma(I)]	R1 = 0.0468, Rw = 0.0411
Absolute structure parameter	UPDATE THIS FIELD
Final maximum delta/sigma	0.000739

Largest diff. peak and hole 0.54 and -0.45 e.A^-3

_____

Comments: UPDATE THIS FIELD IF NECESSARY

Table 2. Selected bond lengths [A] and angles [deg] for MGC50.

Ca(1)-N(5A)	2.4510(16)
Ca(1)-N(3A)	2.4471(16)
Ca(1)-N(1A)	2.4224(16)
Ca(1)-N(1)	2.4224(16)
Ca(1)-N(3)	2.4471(16)
Ca(1)-N(5)	2.4510(16)
N(1)-N(2)	1.373(2)
N(1)-C(1)	1.332(3)
N(2)-C(3)	1.361(2)
N(2)-C(16)	1.446(2)
N(3)-N(4)	1.371(2)
N(3)-C(6)	1.335(3)
N(4)-C(8)	1.362(2)
N(4)-C(16)	1.446(2)
N(5)-N(6)	1.378(2)
N(5)-C(11)	1.330(3)
N(6)-C(13)	1.362(2)
N(6)-C(16)	1.445(2)
B(1)-C(17)	1.650(3)
B(1)-C(23)	1.653(3)
B(1)-C(29)	1.657(3)
B(1)-C(35)	1.657(3)
C(1)-C(2)	1.402(3)
C(1)-C(4)	1.498(3)
C(2)-C(3)	1.368(3)
C(3)-C(5)	1.489(3)
C(6)-C(7)	1.403(3)
C(6)-C(9)	1.494(3)
C(7)-C(8)	1.366(3)
C(8)-C(10)	1.487(3)
C(11)-C(12)	1.401(3)
C(11)-C(14)	1.494(3)
C(12)-C(13)	1.370(3)
C(13)-C(15)	1.493(3)
C(17)-C(18)	1.398(3)
C(17)-C(22)	1.407(3)
C(18)-C(19)	1.398(3)
C(19)-C(20)	1.383(4)
C(20)-C(21)	1.374(4)
C(21)-C(22)	1.393(3)
C(23)-C(24)	1.408(3)
C(23)-C(28)	1.399(3)
C(24)-C(25)	1.386(3)
C(25)-C(26)	1.380(3)
C(26)-C(27)	1.380(3)
C(27)-C(28)	1.390(3)
C(29)-C(30)	1.406(3)
C(29)-C(34)	1.396(3)
C(30)-C(31)	1.391(3)
C(31)-C(32)	1.379(3)
C(32)-C(33)	1.377(3)
C(33)-C(34)	1.398(3)
C(35)-C(36)	1.400(3)
C(35)-C(40)	1.404(3)
C(36)-C(37)	1.392(3)
C(37)-C(38)	1.373(4)
C(38)-C(39)	1.375(4)
C(39)-C(40)	1.388(3)
C(41)-Cl(1)	1.726(3)
C(41)-Cl(2)	1.757(3)

N(5A) -Ca(1)-N(3A)	76.12(5)
N(5A) -Ca(1)-N(1A)	75.96(6)
N(3A) -Ca(1)-N(1A)	75.46(5)
N(5A) -Ca(1)-N(1)	104.04(6)
N(3A) -Ca(1)-N(1)	104.54(5)
N(1A) -Ca(1)-N(1)	179.995
N(5A) -Ca(1)-N(3)	103.88(5)
N(3A) -Ca(1)-N(3)	179.995
N(1A) -Ca(1)-N(3)	104.54(5)
N(1)-Ca(1)-N(3)	75.46(5)
N(5A) -Ca(1)-N(5)	179.995
N(3A) -Ca(1)-N(5)	103.88(5)
N(1A) -Ca(1)-N(5)	104.04(6)
N(1)-Ca(1)-N(5)	75.96(6)
N(3)-Ca(1)-N(5)	76.12(5)
Ca(1)-N(1)-N(2)	120.35(12)
Ca(1)-N(1)-C(1)	134.66(13)
N(2)-N(1)-C(1)	104.95(15)
N(1)-N(2)-C(3)	111.43(15)
N(1)-N(2)-C(16)	121.32(15)
C(3)-N(2)-C(16)	127.22(15)
Ca(1)-N(3)-N(4)	119.90(11)
Ca(1)-N(3)-C(6)	134.58(13)
N(4)-N(3)-C(6)	104.85(15)
N(3)-N(4)-C(8)	111.86(15)
N(3)-N(4)-C(16)	121.08(15)
C(8)-N(4)-C(16)	127.05(15)
Ca(1)-N(5)-N(6)	120.16(12)
Ca(1)-N(5)-C(11)	134.20(13)
N(6)-N(5)-C(11)	104.96(15)
N(5)-N(6)-C(13)	111.75(16)
N(5)-N(6)-C(16)	120.53(14)
C(13)-N(6)-C(16)	127.61(15)
C(17)-B(1)-C(23)	112.21(16)
C(17)-B(1)-C(29)	109.04(16)
C(23)-B(1)-C(29)	110.42(15)
C(17)-B(1)-C(35)	107.69(15)
C(23)-B(1)-C(35)	108.08(15)
C(29)-B(1)-C(35)	109.32(16)
N(1)-C(1)-C(2)	110.97(17)
N(1)-C(1)-C(4)	120.52(19)
C(2)-C(1)-C(4)	128.5(2)
C(1)-C(2)-C(3)	106.12(18)
C(2)-C(3)-N(2)	106.53(17)
C(2)-C(3)-C(5)	130.66(19)
N(2)-C(3)-C(5)	122.79(18)
N(3)-C(6)-C(7)	110.60(17)
N(3)-C(6)-C(9)	120.64(19)
C(7)-C(6)-C(9)	128.76(19)
C(6)-C(7)-C(8)	106.64(18)
C(7)-C(8)-N(4)	106.05(16)
C(7)-C(8)-C(10)	131.17(19)
N(4)-C(8)-C(10)	122.76(18)
N(5)-C(11)-C(12)	110.61(18)
N(5)-C(11)-C(14)	120.37(19)
C(12)-C(11)-C(14)	129.0(2)
C(11)-C(12)-C(13)	106.92(18)
C(12)-C(13)-N(6)	105.75(17)
C(12)-C(13)-C(15)	131.04(19)
N(6)-C(13)-C(15)	123.09(18)
N(2)-C(16)-N(4)	112.50(15)
N(2)-C(16)-N(6)	112.17(15)
N(4)-C(16)-N(6)	112.14(15)

B(1)-C(17)-C(18)	124.78(18)
B(1)-C(17)-C(22)	120.10(19)
C(18)-C(17)-C(22)	115.1(2)
C(17)-C(18)-C(19)	122.8(2)
C(18)-C(19)-C(20)	120.0(3)
C(19)-C(20)-C(21)	119.0(2)
C(20)-C(21)-C(22)	120.6(2)
C(17)-C(22)-C(21)	122.5(2)
B(1)-C(23)-C(24)	121.56(17)
B(1)-C(23)-C(28)	124.35(16)
C(24)-C(23)-C(28)	114.04(18)
C(23)-C(24)-C(25)	123.09(19)
C(24)-C(25)-C(26)	120.51(19)
C(25)-C(26)-C(27)	118.7(2)
C(26)-C(27)-C(28)	120.0(2)
C(23)-C(28)-C(27)	123.66(19)
B(1)-C(29)-C(30)	121.13(17)
B(1)-C(29)-C(34)	123.72(18)
C(30)-C(29)-C(34)	115.15(17)
C(29)-C(30)-C(31)	122.8(2)
C(30)-C(31)-C(32)	120.1(2)
C(31)-C(32)-C(33)	119.11(19)
C(32)-C(33)-C(34)	120.4(2)
C(33)-C(34)-C(29)	122.5(2)
B(1)-C(35)-C(36)	123.89(17)
B(1)-C(35)-C(40)	121.68(18)
C(36)-C(35)-C(40)	114.42(19)
C(35)-C(36)-C(37)	123.0(2)
C(36)-C(37)-C(38)	120.2(2)
C(37)-C(38)-C(39)	119.0(2)
C(38)-C(39)-C(40)	120.4(2)
C(35)-C(40)-C(39)	122.9(2)
Cl(1)-C(41)-Cl(2)	113.28(16)

Symmetry transformations used to generate equivalent atoms:
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;
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_publ_section_exptl_refinement
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C-bound H atoms were placed in calculated positions with reference to
a Fourier difference map. B-bound H atoms were located from a Fourier
difference map and positionally and isotropically refined. Residual
electron density was assigned to a disordered pentane of crystallisation.
This was refined subject to geometric restraints and with a common
isotropic displacement parameter applied to the C atoms.

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_exptl_crystal_density_diffrn     1.070
_exptl_crystal_density_meas       ?
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              2568
_exptl_absorpt_coefficient_mu     0.202

_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_process_details    'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_exptl_absorpt_correction_T_min   0.96
_exptl_absorpt_correction_T_max   0.96
_diffrn_measurement_device_type   'Nonius KappaCCD'
_diffrn_measurement_device        'Area'
_diffrn_radiation_monochromator   'graphite'
_diffrn_radiation_type            'Mo K\a'
_diffrn_radiation_wavelength           0.71073
_diffrn_measurement_method        \w

_computing_data_collection        'COLLECT (Nonius, 2001).'
_computing_cell_refinement        'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_computing_data_reduction         'DENZO/SCALEPACK (Otwinowski & Minor, 1997)'
_computing_structure_solution     'SIR92 (Altomare et al., 1994)'
_computing_structure_refinement   'CRYSTALS (Betteridge et al., 2003)'
_computing_publication_material   'CRYSTALS (Betteridge et al., 2003)'
_computing_molecular_graphics     'CAMERON (Watkin et al., 1996)'

_diffrn_standards_interval_time   .
_diffrn_standards_interval_count  .
_diffrn_standards_number          0
_diffrn_standards_decay_%         ?

_diffrn_ambient_temperature        150
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_diffrn_reflns_number             25981
_reflns_number_total              8257
_diffrn_reflns_av_R_equivalents   0.043


_diffrn_reflns_theta_min          5.095
_diffrn_reflns_theta_max          27.462
_diffrn_measured_fraction_theta_max 0.991

_diffrn_reflns_theta_full         26.912
_diffrn_measured_fraction_theta_full 0.993


_diffrn_reflns_limit_h_min        -26
_diffrn_reflns_limit_h_max        27
_diffrn_reflns_limit_k_min        -20
_diffrn_reflns_limit_k_max        20
_diffrn_reflns_limit_l_min        -28
_diffrn_reflns_limit_l_max        23
_reflns_limit_h_min               -27
_reflns_limit_h_max               26
_reflns_limit_k_min               0
_reflns_limit_k_max               20
_reflns_limit_l_min               0
_reflns_limit_l_max               28

_oxford_diffrn_Wilson_B_factor    2.49
_oxford_diffrn_Wilson_scale       19.46

_atom_sites_solution_primary      Direct
_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens    geom

_refine_diff_density_min          -0.64
_refine_diff_density_max          0.54


# The current dictionary definitions do not cover the
# situation where the reflections used for refinement were
# selected by a user-defined sigma threshold


# The values actually used during refinement
_oxford_reflns_threshold_expression_ref     I>3.0\s(I)
_refine_ls_number_reflns          5311
_refine_ls_number_restraints      4
_refine_ls_number_parameters      376
_oxford_refine_ls_R_factor_ref    0.0510
_refine_ls_wR_factor_ref          0.0609
_refine_ls_goodness_of_fit_ref    1.0901
_refine_ls_shift/su_max           0.0151427
_refine_ls_shift/su_mean          0.0009163


# The values computed from all data
_oxford_reflns_number_all         8257
_refine_ls_R_factor_all           0.0893
_refine_ls_wR_factor_all          0.0867

# The values computed with a 2 sigma cutoff - a la SHELX
_reflns_threshold_expression      I>2.0\s(I)
```

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_reflns_number_gt                 5845
_refine_ls_R_factor_gt            0.0571
_refine_ls_wR_factor_gt           0.0639

_chemical_absolute_configuration  '.'


_refine_ls_structure_factor_coef  F
_refine_ls_matrix_type            full
_refine_ls_hydrogen_treatment     mixed
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 1.88 1.50 1.41
;
_publ_section_references
;
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C.,
Polidori, G. & Camalli, M. (1994). J. Appl. Cryst. 27, 435.

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Otwinowski, Z. & Minor, W. (1997). Methods in Enzymology, Vol. 276,
edited by C. W. Carter Jr & R. M. Sweet, pp. 307--326.
New York: Academic Press.

Prince, E.
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and Materials Science
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Watkin, D.J., Prout, C.K. & Pearce, L.J. (1996). CAMERON, Chemical
Crystallography Laboratory, Oxford, UK.
;

# Uequiv = arithmetic mean of Ui i.e. Ueqiv = (U1+U2+U3)/3



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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_adp_type
_atom_site_refinement_flags_posn
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_atom_site_refinement_flags_occupancy
_atom_site_disorder_assembly
_atom_site_disorder_group
_atom_site_attached_hydrogens
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N1 N 0.44645(8) 0.47785(9) 0.35960(7) 0.0287 1.0000 Uani . . . . . .
N2 N 0.50400(8) 0.50716(9) 0.38734(7) 0.0280 1.0000 Uani . . . . . .
N3 N 0.49186(8) 0.57187(9) 0.25334(7) 0.0293 1.0000 Uani . . . . . .
N4 N 0.54317(7) 0.58649(10) 0.29665(7) 0.0287 1.0000 Uani . . . . . .
N5 N 0.43476(8) 0.66675(10) 0.38675(7) 0.0304 1.0000 Uani . . . . . .
N6 N 0.50047(8) 0.66433(9) 0.38871(7) 0.0294 1.0000 Uani . . . . . .
O1 O 0.39294(6) 0.72626(8) 0.24870(7) 0.0330 1.0000 Uani . . . . . .
C1 C 0.43759(10) 0.40364(11) 0.38552(9) 0.0326 1.0000 Uani . . . . . .
C2 C 0.48832(11) 0.38627(13) 0.43029(10) 0.0379 1.0000 Uani . . . . . .
C3 C 0.52925(10) 0.45244(12) 0.43063(9) 0.0334 1.0000 Uani . . . . . .
C4 C 0.37923(12) 0.35008(13) 0.36694(11) 0.0419 1.0000 Uani . . . . . .
C5 C 0.32164(13) 0.38280(17) 0.39803(15) 0.0560 1.0000 Uani . . . . . .
C6 C 0.36444(14) 0.34787(16) 0.29640(12) 0.0521 1.0000 Uani . . . . . .
C7 C 0.39403(16) 0.26105(15) 0.38972(16) 0.0600 1.0000 Uani . . . . . .
C8 C 0.59060(12) 0.46637(15) 0.47087(11) 0.0447 1.0000 Uani . . . . . .
C9 C 0.51616(11) 0.56393(12) 0.19874(9) 0.0356 1.0000 Uani . . . . . .
C10 C 0.58261(13) 0.57438(13) 0.20654(11) 0.0449 1.0000 Uani . . . . . .
C11 C 0.59842(10) 0.58913(13) 0.26837(11) 0.0387 1.0000 Uani . . . . . .
C12 C 0.47354(15) 0.54181(14) 0.14022(10) 0.0486 1.0000 Uani . . . . . .
C13 C 0.4187(2) 0.60398(19) 0.12827(14) 0.0822 1.0000 Uani . . . . . .
C14 C 0.5135(3) 0.5397(2) 0.08520(15) 0.0912 1.0000 Uani . . . . . .
C15 C 0.44477(15) 0.45573(16) 0.14806(13) 0.0559 1.0000 Uani . . . . . .
C16 C 0.66327(11) 0.60536(19) 0.30179(15) 0.0578 1.0000 Uani . . . . . .
C17 C 0.41974(11) 0.73654(12) 0.41593(9) 0.0353 1.0000 Uani . . . . . .
C18 C 0.47614(13) 0.77915(13) 0.43640(10) 0.0424 1.0000 Uani . . . . . .
C19 C 0.52616(11) 0.73206(12) 0.41831(9) 0.0382 1.0000 Uani . . . . . .
C20 C 0.35161(13) 0.76019(14) 0.42553(11) 0.0461 1.0000 Uani . . . . . .
C21 C 0.34783(18) 0.7695(3) 0.49548(15) 0.0835 1.0000 Uani . . . . . .
C22 C 0.3352(2) 0.8423(2) 0.3927(3) 0.1105 1.0000 Uani . . . . . .
C23 C 0.30453(13) 0.6952(2) 0.40121(15) 0.0620 1.0000 Uani . . . . . .
C24 C 0.59649(14) 0.74907(15) 0.42700(14) 0.0545 1.0000 Uani . . . . . .
C25 C 0.45105(10) 0.77523(13) 0.25248(11) 0.0375 1.0000 Uani . . . . . .
C26 C 0.43152(13) 0.85911(14) 0.22702(12) 0.0475 1.0000 Uani . . . . . .
C27 C 0.37673(13) 0.83915(15) 0.17884(14) 0.0529 1.0000 Uani . . . . . .
C28 C 0.34344(11) 0.76820(14) 0.20826(12) 0.0450 1.0000 Uani . . . . . .
B1 B 0.27459(13) 0.55735(18) 0.25116(17) 0.0527 1.0000 Uani . . . . . .
B2 B 0.53691(10) 0.58695(13) 0.36737(10) 0.0285 1.0000 Uani . . . . . .
C29 C 0.2648(6) 0.3653(7) 0.1368(5) 0.1256(14) 0.5000 Uiso D . . . . .
C30 C 0.2375(3) 0.4275(4) 0.0876(3) 0.1256(14) 1.0000 Uiso D . . . . .
C31 C 0.2594(6) 0.4036(8) 0.0256(4) 0.1256(14) 0.5000 Uiso D . . . . .
C311 C 0.2667(6) 0.4606(8) 0.0296(4) 0.1256(14) 0.5000 Uiso D . . . . .
H1 H 0.2208(18) 0.537(2) 0.2368(18) 0.082(11) 1.0000 Uiso . . . . . .
H2 H 0.308(2) 0.530(2) 0.2211(19) 0.088(12) 1.0000 Uiso . . . . . .
H3 H 0.2828(17) 0.540(2) 0.3039(18) 0.074(10) 1.0000 Uiso . . . . . .
H4 H 0.2828(13) 0.6264(18) 0.2536(13) 0.050(7) 1.0000 Uiso . . . . . .
H5 H 0.5850(11) 0.5877(13) 0.3898(11) 0.030(5) 1.0000 Uiso . . . . . .
H21 H 0.4936 0.3376 0.4555 0.0460 1.0000 Uiso . . . . . .
H51 H 0.3129 0.4382 0.3851 0.0694 1.0000 Uiso R . . . . .
H52 H 0.2852 0.3492 0.3865 0.0694 1.0000 Uiso R . . . . .
H53 H 0.3312 0.3813 0.4418 0.0694 1.0000 Uiso R . . . . .
H61 H 0.3560 0.4024 0.2814 0.0650 1.0000 Uiso R . . . . .
H62 H 0.3279 0.3141 0.2858 0.0650 1.0000 Uiso R . . . . .
H63 H 0.4003 0.3258 0.2781 0.0650 1.0000 Uiso R . . . . .
H71 H 0.3579 0.2267 0.3785 0.0749 1.0000 Uiso R . . . . .
H72 H 0.4032 0.2610 0.4336 0.0749 1.0000 Uiso R . . . . .
```

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H73 H 0.4301 0.2406 0.3710 0.0749 1.0000 Uiso R . . . . .
H81 H 0.5990 0.4203 0.4977 0.0552 1.0000 Uiso R . . . . .
H82 H 0.6249 0.4729 0.4455 0.0552 1.0000 Uiso R . . . . .
H83 H 0.5868 0.5150 0.4950 0.0552 1.0000 Uiso R . . . . .
H101 H 0.6113 0.5719 0.1751 0.0541 1.0000 Uiso R . . . . .
H131 H 0.3929 0.5889 0.0915 0.1023 1.0000 Uiso R . . . . .
H132 H 0.4355 0.6581 0.1236 0.1023 1.0000 Uiso R . . . . .
H133 H 0.3934 0.6032 0.1624 0.1023 1.0000 Uiso R . . . . .
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H142 H 0.5462 0.4992 0.0926 0.1100 1.0000 Uiso R . . . . .
H143 H 0.5325 0.5924 0.0802 0.1100 1.0000 Uiso R . . . . .
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H152 H 0.4783 0.4161 0.1550 0.0697 1.0000 Uiso R . . . . .
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H162 H 0.6727 0.5637 0.3323 0.0712 1.0000 Uiso R . . . . .
H163 H 0.6949 0.6046 0.2731 0.0712 1.0000 Uiso R . . . . .
H181 H 0.4793 0.8302 0.4582 0.0517 1.0000 Uiso R . . . . .
H211 H 0.3054 0.7844 0.5032 0.1033 1.0000 Uiso R . . . . .
H212 H 0.3769 0.8115 0.5110 0.1033 1.0000 Uiso R . . . . .
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H221 H 0.3397 0.8370 0.3496 0.1329 1.0000 Uiso R . . . . .
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H223 H 0.3639 0.8836 0.4101 0.1329 1.0000 Uiso R . . . . .
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H242 H 0.6176 0.7053 0.4500 0.0678 1.0000 Uiso R . . . . .
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H251 H 0.4688 0.7797 0.2944 0.0465 1.0000 Uiso R . . . . .
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H261 H 0.4658 0.8851 0.2088 0.0589 1.0000 Uiso R . . . . .
H262 H 0.4176 0.8938 0.2586 0.0589 1.0000 Uiso R . . . . .
H271 H 0.3487 0.8851 0.1717 0.0652 1.0000 Uiso R . . . . .
H272 H 0.3922 0.8228 0.1408 0.0652 1.0000 Uiso R . . . . .
H281 H 0.3253 0.7313 0.1772 0.0558 1.0000 Uiso R . . . . .
H282 H 0.3106 0.7884 0.2317 0.0558 1.0000 Uiso R . . . . .
H291 H 0.3104 0.3674 0.1410 0.1606 0.5000 Uiso R . . . . .
H292 H 0.2491 0.3794 0.1752 0.1606 0.5000 Uiso R . . . . .
H293 H 0.2511 0.3109 0.1251 0.1606 0.5000 Uiso R . . . . .
H301 H 0.2286 0.4759 0.1102 0.1606 0.5000 Uiso R . . . . .
H302 H 0.1983 0.4034 0.0706 0.1606 0.5000 Uiso R . . . . .
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H304 H 0.2516 0.4821 0.0980 0.1517 0.5000 Uiso R . . . . .
H305 H 0.1919 0.4253 0.0856 0.1517 0.5000 Uiso R . . . . .
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N1 0.0323(8) 0.0223(7) 0.0306(8) 0.0017(6) -0.0009(6) 0.0010(6)
N2 0.0318(8) 0.0244(7) 0.0272(8) 0.0010(6) 0.0000(6) 0.0035(6)
```

```
N3 0.0335(8) 0.0273(7) 0.0266(7) 0.0006(6) 0.0005(6) 0.0064(6)
N4 0.0258(7) 0.0281(7) 0.0322(8) 0.0025(6) 0.0033(6) 0.0050(6)
N5 0.0399(9) 0.0268(7) 0.0245(7) -0.0024(6) 0.0041(6) 0.0042(6)
N6 0.0365(8) 0.0239(7) 0.0274(8) -0.0009(6) 0.0005(6) -0.0022(6)
O1 0.0308(6) 0.0241(6) 0.0430(8) 0.0057(5) -0.0015(6) 0.0000(5)
C1 0.0414(10) 0.0222(8) 0.0344(9) 0.0030(7) 0.0051(8) 0.0041(8)
C2 0.0481(12) 0.0298(9) 0.0358(11) 0.0099(8) 0.0042(9) 0.0077(8)
C3 0.0387(10) 0.0317(9) 0.0291(9) 0.0033(7) 0.0006(8) 0.0104(8)
C4 0.0487(12) 0.0258(9) 0.0509(13) 0.0038(9) 0.0035(10) -0.0061(9)
C5 0.0437(13) 0.0498(14) 0.0752(18) 0.0015(13) 0.0099(12) -0.0086(11)
C6 0.0587(14) 0.0425(12) 0.0526(14) -0.0032(10) -0.0068(11) -0.0128(11)
C7 0.0739(18) 0.0276(11) 0.0770(19) 0.0107(11) 0.0001(14) -0.0056(11)
C8 0.0461(12) 0.0467(12) 0.0389(11) 0.0101(9) -0.0080(9) 0.0080(10)
C9 0.0541(12) 0.0242(9) 0.0293(9) 0.0023(7) 0.0087(8) 0.0107(8)
C10 0.0584(14) 0.0336(11) 0.0472(13) 0.0034(9) 0.0276(11) 0.0102(9)
C11 0.0326(10) 0.0337(10) 0.0520(12) 0.0036(9) 0.0151(9) 0.0067(8)
C12 0.0852(18) 0.0326(11) 0.0277(10) -0.0034(8) 0.0037(10) 0.0114(11)
C13 0.139(3) 0.0513(16) 0.0471(15) -0.0119(12) -0.0396(18) 0.0377(18)
C14 0.168(4) 0.074(2) 0.0364(14) -0.0118(14) 0.0314(19) -0.021(2)
C15 0.0772(18) 0.0412(13) 0.0463(13) -0.0057(10) -0.0098(12) 0.0028(12)
C16 0.0295(10) 0.0618(16) 0.084(2) -0.0023(14) 0.0151(11) 0.0009(10)
C17 0.0555(12) 0.0257(9) 0.0251(9) -0.0002(7) 0.0062(8) 0.0083(8)
C18 0.0687(15) 0.0238(9) 0.0342(11) -0.0042(8) 0.0022(10) -0.0003(9)
C19 0.0553(13) 0.0276(9) 0.0305(10) -0.0004(8) -0.0019(9) -0.0066(9)
C20 0.0634(15) 0.0388(11) 0.0378(11) -0.0030(9) 0.0140(10) 0.0178(10)
C21 0.078(2) 0.122(3) 0.0544(18) -0.0374(19) 0.0259(16) 0.000(2)
C22 0.111(3) 0.070(2) 0.161(4) 0.054(3) 0.068(3) 0.059(2)
C23 0.0451(13) 0.0734(18) 0.0659(17) -0.0208(14) -0.0024(12) 0.0209(13)
C24 0.0598(15) 0.0379(12) 0.0633(16) -0.0061(11) -0.0076(12) -0.0160(11)
C25 0.0366(10) 0.0294(10) 0.0452(11) 0.0042(8) -0.0020(8) -0.0070(8)
C26 0.0572(14) 0.0311(10) 0.0548(14) 0.0055(9) 0.0073(11) -0.0095(10)
C27 0.0535(14) 0.0376(12) 0.0667(16) 0.0214(11) 0.0008(12) 0.0005(10)
C28 0.0351(10) 0.0317(10) 0.0665(15) 0.0164(10) -0.0043(10) 0.0045(8)
B1 0.0338(13) 0.0392(14) 0.081(2) 0.0025(13) -0.0152(13) -0.0055(11)
B2 0.0274(9) 0.0266(9) 0.0306(10) -0.0008(8) -0.0027(7) 0.0024(8)

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Ca1 . N3 . 2.4256(17)    yes
Ca1 . N5 . 2.4307(16)    yes
Ca1 . O1 . 2.4291(14)    yes
Ca1 . H2 . 2.44(4)    no
Ca1 . H3 . 2.40(3)    no
Ca1 . H4 . 2.41(3)    no
N1 . N2 . 1.377(2)    yes
N1 . C1 . 1.344(2)    yes
N2 . C3 . 1.358(2)    yes
N2 . B2 . 1.543(3)    yes
N3 . N4 . 1.376(2)    yes
N3 . C9 . 1.337(3)    yes
N4 . C11 . 1.360(3)    yes
N4 . B2 . 1.549(3)    yes
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N5 . N6 . 1.372(2)    yes
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_diffrn_reflns_theta_max          27.458
_diffrn_measured_fraction_theta_max 0.985

_diffrn_reflns_theta_full         26.085
_diffrn_measured_fraction_theta_full 0.990


_diffrn_reflns_limit_h_min        -15
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_diffrn_reflns_limit_k_min        -20
_diffrn_reflns_limit_k_max        20
_diffrn_reflns_limit_l_min        -22
_diffrn_reflns_limit_l_max        22
_reflns_limit_h_min               -15
_reflns_limit_h_max               15
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_reflns_limit_k_max               20
_reflns_limit_l_min               0
_reflns_limit_l_max               22

_oxford_diffrn_Wilson_B_factor    3.62
_oxford_diffrn_Wilson_scale       5.19

_atom_sites_solution_primary      Direct
_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens    geom

_refine_diff_density_min          -0.91
_refine_diff_density_max          0.92


# The current dictionary definitions do not cover the
# situation where the reflections used for refinement were
# selected by a user-defined sigma threshold


# The values actually used during refinement
_oxford_reflns_threshold_expression_ref     I>3.0\s(I)
_refine_ls_number_reflns          6192
_refine_ls_number_restraints      0
_refine_ls_number_parameters      348
_oxford_refine_ls_R_factor_ref    0.0475
_refine_ls_wR_factor_ref          0.0527
_refine_ls_goodness_of_fit_ref    1.1013
_refine_ls_shift/su_max           0.0010045
```

```
_refine_ls_shift/su_mean          0.0000209


# The values computed from all data
_oxford_reflns_number_all         7416
_refine_ls_R_factor_all           0.0581
_refine_ls_wR_factor_all          0.0631

# The values computed with a 2 sigma cutoff - a la SHELX
_reflns_threshold_expression      I>2.0\s(I)
_reflns_number_gt                 6546
_refine_ls_R_factor_gt            0.0496
_refine_ls_wR_factor_gt           0.0541

_refine_ls_abs_structure_Flack    0.015(19)
_refine_ls_abs_structure_details  'Flack (1983), 3249 Friedel-pairs'
_chemical_absolute_configuration  'ad'


_refine_ls_structure_factor_coef  F
_refine_ls_matrix_type            full
_refine_ls_hydrogen_treatment     mixed
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
;
 Method, part 1, Chebychev polynomial, (Watkin, 1994, Prince, 1982)
 [weight] = 1.0/[A~0~*T~0~(x)+A~1~*T~1~(x) ... +A~n-1~]*T~n-1~(x)]
 where A~i~ are the Chebychev coefficients listed below and x= Fcalc/Fmax
 Method = Robust Weighting (Prince, 1982)
 W = [weight] * [1-(deltaF/6*sigmaF)^2^]^2^
 A~i~ are:
 1.90 0.953 1.50
;
_publ_section_references
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Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M.C.,
Polidori, G. & Camalli, M. (1994). J. Appl. Cryst. 27, 435.

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Crystallography Laboratory, Oxford, UK.
;
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# Uequiv = arithmetic mean of Ui i.e. Ueqiv = (U1+U2+U3)/3



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_atom_site_adp_type
_atom_site_refinement_flags_posn
_atom_site_refinement_flags_adp
_atom_site_refinement_flags_occupancy
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_atom_site_disorder_group
_atom_site_attached_hydrogens
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I1 I 0.19705(2) 0.733876(18) 0.255116(15) 0.0540 1.0000 Uani . . . . . .
O1 O 0.3302(2) 0.51169(16) 0.22593(14) 0.0406 1.0000 Uani . . . . . .
N1 N 0.5272(2) 0.5635(2) 0.33436(18) 0.0360 1.0000 Uani . . . . . .
N2 N 0.5482(2) 0.49951(19) 0.38755(17) 0.0332 1.0000 Uani . . . . . .
N3 N 0.2881(2) 0.47308(19) 0.40894(16) 0.0337 1.0000 Uani . . . . . .
N4 N 0.3730(2) 0.43903(19) 0.45030(17) 0.0348 1.0000 Uani . . . . . .
N5 N 0.3997(2) 0.63842(19) 0.46881(16) 0.0316 1.0000 Uani . . . . . .
N6 N 0.4598(2) 0.5746(2) 0.50209(16) 0.0341 1.0000 Uani . . . . . .
C1 C 0.6068(3) 0.5603(2) 0.2822(2) 0.0381 1.0000 Uani . . . . . .
C2 C 0.6791(3) 0.4925(3) 0.2988(2) 0.0455 1.0000 Uani . . . . . .
C3 C 0.6403(3) 0.4561(3) 0.3666(2) 0.0420 1.0000 Uani . . . . . .
C4 C 0.6155(3) 0.6223(3) 0.2154(2) 0.0406 1.0000 Uani . . . . . .
C5 C 0.5229(4) 0.6885(3) 0.2172(3) 0.0572 1.0000 Uani . . . . . .
C6 C 0.6108(5) 0.5731(4) 0.1393(3) 0.0577 1.0000 Uani . . . . . .
C7 C 0.7264(4) 0.6691(4) 0.2195(3) 0.0598 1.0000 Uani . . . . . .
C8 C 0.6850(4) 0.3829(3) 0.4118(3) 0.0538 1.0000 Uani . . . . . .
C9 C 0.2031(3) 0.4196(2) 0.41495(19) 0.0370 1.0000 Uani . . . . . .
C10 C 0.2357(4) 0.3482(3) 0.4600(3) 0.0479 1.0000 Uani . . . . . .
C11 C 0.3413(3) 0.3633(2) 0.4810(2) 0.0409 1.0000 Uani . . . . . .
C12 C 0.0936(3) 0.4345(3) 0.3783(2) 0.0407 1.0000 Uani . . . . . .
C13 C 0.0052(4) 0.4329(4) 0.4412(3) 0.0521 1.0000 Uani . . . . . .
C14 C 0.0709(4) 0.3621(4) 0.3214(3) 0.0627 1.0000 Uani . . . . . .
C15 C 0.0895(3) 0.5201(3) 0.3377(3) 0.0527 1.0000 Uani . . . . . .
C16 C 0.4137(4) 0.3082(3) 0.5310(3) 0.0621 1.0000 Uani . . . . . .
C17 C 0.3956(3) 0.7026(2) 0.5202(2) 0.0347 1.0000 Uani . . . . . .
C18 C 0.4535(3) 0.6804(3) 0.5868(2) 0.0387 1.0000 Uani . . . . . .
C19 C 0.4930(3) 0.5990(3) 0.5736(2) 0.0371 1.0000 Uani . . . . . .
C20 C 0.3377(3) 0.7860(2) 0.5027(2) 0.0421 1.0000 Uani . . . . . .
C21 C 0.2152(3) 0.7691(3) 0.4873(3) 0.0520 1.0000 Uani . . . . . .
C22 C 0.3888(4) 0.8280(3) 0.4315(3) 0.0588 1.0000 Uani . . . . . .
C23 C 0.3477(6) 0.8458(4) 0.5709(4) 0.0748 1.0000 Uani . . . . . .
C24 C 0.5627(4) 0.5453(3) 0.6253(3) 0.0507 1.0000 Uani . . . . . .
C25 C 0.3756(3) 0.4252(2) 0.2292(2) 0.0422 1.0000 Uani . . . . . .
C26 C 0.3260(3) 0.3781(3) 0.1616(2) 0.0432 1.0000 Uani . . . . . .
C27 C 0.3126(4) 0.4493(3) 0.1026(2) 0.0453 1.0000 Uani . . . . . .
C28 C 0.2781(4) 0.5237(3) 0.1503(2) 0.0497 1.0000 Uani . . . . . .
B1 B 0.4823(3) 0.4875(3) 0.4637(2) 0.0342 1.0000 Uani . . . . . .
H1 H 0.526(4) 0.442(3) 0.500(2) 0.035(10) 1.0000 Uiso . . . . . .
H21 H 0.7413 0.4752 0.2699 0.0544 1.0000 Uiso R . . . . .
H51 H 0.5304 0.7268 0.1750 0.0719 1.0000 Uiso R . . . . .
H52 H 0.4547 0.6598 0.2138 0.0719 1.0000 Uiso R . . . . .
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H53 H 0.5261 0.7198 0.2641 0.0719 1.0000 Uiso R . . . . .
H61 H 0.6165 0.6121 0.0975 0.0712 1.0000 Uiso R . . . . .
H62 H 0.5433 0.5432 0.1361 0.0712 1.0000 Uiso R . . . . .
H63 H 0.6695 0.5334 0.1372 0.0712 1.0000 Uiso R . . . . .
H71 H 0.7319 0.7081 0.1777 0.0741 1.0000 Uiso R . . . . .
H72 H 0.7846 0.6290 0.2169 0.0741 1.0000 Uiso R . . . . .
H73 H 0.7304 0.6996 0.2668 0.0741 1.0000 Uiso R . . . . .
H81 H 0.6406 0.3731 0.4559 0.0644 1.0000 Uiso R . . . . .
H82 H 0.6851 0.3331 0.3803 0.0644 1.0000 Uiso R . . . . .
H83 H 0.7576 0.3953 0.4276 0.0644 1.0000 Uiso R . . . . .
H101 H 0.1921 0.3000 0.4730 0.0592 1.0000 Uiso R . . . . .
H131 H -0.0647 0.4424 0.4189 0.0622 1.0000 Uiso R . . . . .
H132 H 0.0061 0.3787 0.4659 0.0622 1.0000 Uiso R . . . . .
H133 H 0.0199 0.4765 0.4780 0.0622 1.0000 Uiso R . . . . .
H141 H 0.0017 0.3707 0.2978 0.0787 1.0000 Uiso R . . . . .
H142 H 0.0705 0.3093 0.3486 0.0787 1.0000 Uiso R . . . . .
H143 H 0.1262 0.3607 0.2830 0.0787 1.0000 Uiso R . . . . .
H151 H 0.0195 0.5279 0.3151 0.0649 1.0000 Uiso R . . . . .
H152 H 0.1439 0.5219 0.2986 0.0649 1.0000 Uiso R . . . . .
H153 H 0.1027 0.5644 0.3740 0.0649 1.0000 Uiso R . . . . .
H161 H 0.4836 0.3342 0.5359 0.0755 1.0000 Uiso R . . . . .
H162 H 0.4214 0.2533 0.5081 0.0755 1.0000 Uiso R . . . . .
H163 H 0.3814 0.3025 0.5805 0.0755 1.0000 Uiso R . . . . .
H181 H 0.4635 0.7141 0.6318 0.0470 1.0000 Uiso R . . . . .
H211 H 0.1798 0.8218 0.4763 0.0650 1.0000 Uiso R . . . . .
H212 H 0.2080 0.7317 0.4444 0.0650 1.0000 Uiso R . . . . .
H213 H 0.1827 0.7436 0.5313 0.0650 1.0000 Uiso R . . . . .
H221 H 0.3520 0.8803 0.4209 0.0712 1.0000 Uiso R . . . . .
H222 H 0.3819 0.7907 0.3886 0.0712 1.0000 Uiso R . . . . .
H223 H 0.4640 0.8392 0.4410 0.0712 1.0000 Uiso R . . . . .
H231 H 0.3114 0.8982 0.5599 0.0917 1.0000 Uiso R . . . . .
H232 H 0.3156 0.8200 0.6149 0.0917 1.0000 Uiso R . . . . .
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H271 H 0.2581 0.4352 0.0658 0.0544 1.0000 Uiso R . . . . .
H272 H 0.3796 0.4609 0.0769 0.0544 1.0000 Uiso R . . . . .
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I1 0.06778(17) 0.04998(15) 0.04414(14) 0.00692(11) -0.00233(12) 0.02285(11)
O1 0.0530(14) 0.0353(12) 0.0335(11) -0.0050(9) -0.0088(10) 0.0065(11)
N1 0.0359(14) 0.0374(15) 0.0347(14) 0.0000(12) 0.0014(12) 0.0014(12)
N2 0.0331(14) 0.0327(14) 0.0338(13) 0.0000(11) -0.0006(11) 0.0038(11)
N3 0.0359(15) 0.0341(14) 0.0311(12) -0.0005(10) -0.0014(11) -0.0040(12)
N4 0.0432(15) 0.0299(14) 0.0313(14) -0.0004(11) 0.0015(11) -0.0008(12)
N5 0.0326(13) 0.0314(13) 0.0307(13) -0.0021(11) -0.0016(11) -0.0007(10)
N6 0.0333(13) 0.0375(14) 0.0316(13) -0.0005(11) -0.0009(11) 0.0025(11)
```

```
C1 0.0346(16) 0.0422(19) 0.0375(16) -0.0043(14) -0.0003(13) -0.0029(14)
C2 0.041(2) 0.050(2) 0.0461(18) -0.0046(16) 0.0075(16) 0.0056(16)
C3 0.0391(18) 0.0423(19) 0.0447(19) -0.0018(15) -0.0005(14) 0.0047(15)
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C5 0.065(3) 0.053(2) 0.054(2) 0.013(2) 0.010(2) 0.006(2)
C6 0.069(3) 0.068(3) 0.0369(19) -0.0073(19) 0.0049(18) -0.008(2)
C7 0.059(3) 0.066(3) 0.054(2) 0.011(2) 0.003(2) -0.019(2)
C8 0.052(2) 0.052(2) 0.058(2) 0.0017(18) 0.0101(19) 0.0209(19)
C9 0.0453(18) 0.0342(16) 0.0314(14) 0.0006(12) 0.0053(14) -0.0045(14)
C10 0.051(2) 0.040(2) 0.053(2) 0.0078(17) 0.0085(17) -0.0073(16)
C11 0.0490(19) 0.0304(15) 0.0432(18) 0.0066(14) 0.0045(15) 0.0028(15)
C12 0.0391(18) 0.045(2) 0.0378(17) -0.0067(16) 0.0016(14) -0.0086(15)
C13 0.042(2) 0.065(3) 0.049(2) 0.003(2) 0.0100(17) -0.0091(19)
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C15 0.0390(19) 0.062(3) 0.057(2) 0.011(2) -0.0037(18) -0.0076(18)
C16 0.067(3) 0.045(2) 0.075(3) 0.028(2) 0.002(2) 0.008(2)
C17 0.0349(16) 0.0360(16) 0.0332(15) -0.0037(13) 0.0029(13) -0.0041(13)
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C19 0.0339(16) 0.047(2) 0.0303(16) -0.0034(14) -0.0028(12) -0.0030(15)
C20 0.0473(19) 0.0359(18) 0.0430(17) -0.0025(14) 0.0068(15) 0.0020(15)
C21 0.045(2) 0.048(2) 0.063(2) 0.011(2) 0.0044(17) 0.0125(18)
C22 0.068(3) 0.038(2) 0.071(3) 0.011(2) 0.013(2) -0.004(2)
C23 0.094(4) 0.055(3) 0.076(3) -0.032(3) -0.007(3) 0.015(3)
C24 0.048(2) 0.060(3) 0.044(2) 0.0002(19) -0.0123(17) 0.0085(19)
C25 0.052(2) 0.0359(17) 0.0384(18) -0.0034(14) -0.0039(14) 0.0054(15)
C26 0.049(2) 0.0428(19) 0.0377(16) -0.0099(15) 0.0016(15) -0.0008(15)
C27 0.052(2) 0.052(2) 0.0317(15) -0.0037(15) -0.0022(16) -0.0069(19)
C28 0.065(3) 0.046(2) 0.0379(18) -0.0001(16) -0.0109(17) 0.0079(18)
B1 0.0400(19) 0.0301(17) 0.0325(18) 0.0018(14) -0.0019(14) 0.0000(14)

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Ca1 . O1 . 2.402(2)    yes
Ca1 . N1 . 2.413(3)    yes
Ca1 . N3 . 2.440(3)    yes
Ca1 . N5 . 2.471(3)    yes
O1 . C25 . 1.462(5)    yes
O1 . C28 . 1.471(5)    yes
N1 . N2 . 1.385(4)    yes
N1 . C1 . 1.330(5)    yes
N2 . C3 . 1.364(5)    yes
N2 . B1 . 1.560(5)    yes
N3 . N4 . 1.370(4)    yes
N3 . C9 . 1.337(5)    yes
N4 . C11 . 1.354(5)    yes
N4 . B1 . 1.553(5)    yes
N5 . N6 . 1.367(4)    yes
N5 . C17 . 1.344(5)    yes
N6 . C19 . 1.361(5)    yes
N6 . B1 . 1.540(5)    yes
C1 . C2 . 1.409(6)    yes
C1 . C4 . 1.514(5)    yes
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C2 . C3 . 1.391(6) yes
C2 . H21 . 0.950 no
C3 . C8 . 1.491(6) yes
C4 . C5 . 1.534(6) yes
C4 . C6 . 1.528(6) yes
C4 . C7 . 1.542(6) yes
C5 . H51 . 0.950 no
C5 . H52 . 0.950 no
C5 . H53 . 0.950 no
C6 . H61 . 0.950 no
C6 . H62 . 0.950 no
C6 . H63 . 0.950 no
C7 . H71 . 0.950 no
C7 . H72 . 0.950 no
C7 . H73 . 0.950 no
C8 . H81 . 0.950 no
C8 . H82 . 0.950 no
C8 . H83 . 0.950 no
C9 . C10 . 1.419(6) yes
C9 . C12 . 1.501(6) yes
C10 . C11 . 1.363(6) yes
C10 . H101 . 0.950 no
C11 . C16 . 1.508(6) yes
C12 . C13 . 1.537(5) yes
C12 . C14 . 1.526(6) yes
C12 . C15 . 1.513(6) yes
C13 . H131 . 0.950 no
C13 . H132 . 0.950 no
C13 . H133 . 0.950 no
C14 . H141 . 0.950 no
C14 . H142 . 0.950 no
C14 . H143 . 0.950 no
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C15 . H152 . 0.950 no
C15 . H153 . 0.950 no
C16 . H161 . 0.950 no
C16 . H162 . 0.950 no
C16 . H163 . 0.950 no
C17 . C18 . 1.398(5) yes
C17 . C20 . 1.513(5) yes
C18 . C19 . 1.379(6) yes
C18 . H181 . 0.950 no
C19 . C24 . 1.495(6) yes
C20 . C21 . 1.545(6) yes
C20 . C22 . 1.532(6) yes
C20 . C23 . 1.512(6) yes
C21 . H211 . 0.950 no
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C21 . H213 . 0.950 no
C22 . H221 . 0.950 no
C22 . H222 . 0.950 no
C22 . H223 . 0.950 no
C23 . H231 . 0.950 no
C23 . H232 . 0.950 no
C23 . H233 . 0.950 no
C24 . H241 . 0.950 no
C24 . H242 . 0.950 no
C24 . H243 . 0.950 no
C25 . C26 . 1.511(5) yes
C25 . H251 . 0.950 no
C25 . H252 . 0.950 no

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C26 . C27 . 1.521(6)    yes
C26 . H261 . 0.950    no
C26 . H262 . 0.950    no
C27 . C28 . 1.487(6)    yes
C27 . H271 . 0.950    no
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O1 . Ca1 . N1 . 82.10(10)    yes
I1 . Ca1 . N3 . 131.71(8)    yes
O1 . Ca1 . N3 . 85.09(9)    yes
N1 . Ca1 . N3 . 92.16(11)    yes
I1 . Ca1 . N5 . 117.26(7)    yes
O1 . Ca1 . N5 . 152.62(10)    yes
N1 . Ca1 . N5 . 77.00(10)    yes
N3 . Ca1 . N5 . 78.28(10)    yes
Ca1 . O1 . C25 . 120.1(2)    yes
Ca1 . O1 . C28 . 131.2(2)    yes
C25 . O1 . C28 . 108.5(3)    yes
Ca1 . N1 . N2 . 110.2(2)    yes
Ca1 . N1 . C1 . 137.2(2)    yes
N2 . N1 . C1 . 106.9(3)    yes
N1 . N2 . C3 . 109.5(3)    yes
N1 . N2 . B1 . 123.8(3)    yes
C3 . N2 . B1 . 126.3(3)    yes
Ca1 . N3 . N4 . 113.8(2)    yes
Ca1 . N3 . C9 . 138.1(2)    yes
N4 . N3 . C9 . 107.8(3)    yes
N3 . N4 . C11 . 109.2(3)    yes
N3 . N4 . B1 . 122.8(3)    yes
C11 . N4 . B1 . 127.7(3)    yes
Ca1 . N5 . N6 . 113.1(2)    yes
Ca1 . N5 . C17 . 140.4(2)    yes
N6 . N5 . C17 . 106.5(3)    yes
N5 . N6 . C19 . 110.0(3)    yes
N5 . N6 . B1 . 123.9(3)    yes
C19 . N6 . B1 . 126.1(3)    yes
N1 . C1 . C2 . 110.4(3)    yes
N1 . C1 . C4 . 123.3(3)    yes
C2 . C1 . C4 . 126.3(3)    yes
C1 . C2 . C3 . 105.5(3)    yes
C1 . C2 . H21 . 127.5    no
C3 . C2 . H21 . 127.1    no
C2 . C3 . N2 . 107.7(3)    yes
C2 . C3 . C8 . 129.3(4)    yes
N2 . C3 . C8 . 123.0(4)    yes
C1 . C4 . C5 . 111.3(3)    yes
C1 . C4 . C6 . 109.7(4)    yes
C5 . C4 . C6 . 109.2(4)    yes
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C1 . C4 . C7 . 109.2(3)    yes
C5 . C4 . C7 . 109.1(4)    yes
C6 . C4 . C7 . 108.2(4)    yes
C4 . C5 . H51 . 109.7    no
C4 . C5 . H52 . 109.2    no
H51 . C5 . H52 . 109.5    no
C4 . C5 . H53 . 109.5    no
H51 . C5 . H53 . 109.5    no
H52 . C5 . H53 . 109.5    no
C4 . C6 . H61 . 109.6    no
C4 . C6 . H62 . 109.4    no
H61 . C6 . H62 . 109.5    no
C4 . C6 . H63 . 109.5    no
H61 . C6 . H63 . 109.5    no
H62 . C6 . H63 . 109.5    no
C4 . C7 . H71 . 109.3    no
C4 . C7 . H72 . 110.2    no
H71 . C7 . H72 . 109.5    no
C4 . C7 . H73 . 108.9    no
H71 . C7 . H73 . 109.5    no
H72 . C7 . H73 . 109.5    no
C3 . C8 . H81 . 109.7    no
C3 . C8 . H82 . 109.0    no
H81 . C8 . H82 . 109.5    no
C3 . C8 . H83 . 109.8    no
H81 . C8 . H83 . 109.5    no
H82 . C8 . H83 . 109.5    no
N3 . C9 . C10 . 108.4(3)    yes
N3 . C9 . C12 . 124.3(3)    yes
C10 . C9 . C12 . 127.3(3)    yes
C9 . C10 . C11 . 106.1(4)    yes
C9 . C10 . H101 . 126.6    no
C11 . C10 . H101 . 127.2    no
C10 . C11 . N4 . 108.4(4)    yes
C10 . C11 . C16 . 127.7(4)    yes
N4 . C11 . C16 . 123.8(4)    yes
C9 . C12 . C13 . 108.9(3)    yes
C9 . C12 . C14 . 108.8(4)    yes
C13 . C12 . C14 . 108.7(4)    yes
C9 . C12 . C15 . 111.3(3)    yes
C13 . C12 . C15 . 108.8(4)    yes
C14 . C12 . C15 . 110.3(4)    yes
C12 . C13 . H131 . 109.9    no
C12 . C13 . H132 . 109.1    no
H131 . C13 . H132 . 109.5    no
C12 . C13 . H133 . 109.5    no
H131 . C13 . H133 . 109.5    no
H132 . C13 . H133 . 109.5    no
C12 . C14 . H141 . 109.6    no
C12 . C14 . H142 . 108.8    no
H141 . C14 . H142 . 109.5    no
C12 . C14 . H143 . 109.9    no
H141 . C14 . H143 . 109.5    no
H142 . C14 . H143 . 109.5    no
C12 . C15 . H151 . 109.6    no
C12 . C15 . H152 . 109.6    no
H151 . C15 . H152 . 109.5    no
C12 . C15 . H153 . 109.2    no
H151 . C15 . H153 . 109.5    no
H152 . C15 . H153 . 109.5    no
C11 . C16 . H161 . 109.6    no
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C11 . C16 . H162 . 109.5    no
H161 . C16 . H162 . 109.5    no
C11 . C16 . H163 . 109.3    no
H161 . C16 . H163 . 109.5    no
H162 . C16 . H163 . 109.5    no
N5 . C17 . C18 . 110.2(3)    yes
N5 . C17 . C20 . 121.7(3)    yes
C18 . C17 . C20 . 128.0(3)    yes
C17 . C18 . C19 . 105.6(3)    yes
C17 . C18 . H181 . 127.4    no
C19 . C18 . H181 . 127.0    no
C18 . C19 . N6 . 107.8(3)    yes
C18 . C19 . C24 . 128.2(3)    yes
N6 . C19 . C24 . 124.0(4)    yes
C17 . C20 . C21 . 109.9(3)    yes
C17 . C20 . C22 . 109.9(3)    yes
C21 . C20 . C22 . 109.2(4)    yes
C17 . C20 . C23 . 109.6(4)    yes
C21 . C20 . C23 . 108.6(4)    yes
C22 . C20 . C23 . 109.5(4)    yes
C20 . C21 . H211 . 109.2    no
C20 . C21 . H212 . 109.3    no
H211 . C21 . H212 . 109.5    no
C20 . C21 . H213 . 109.8    no
H211 . C21 . H213 . 109.5    no
H212 . C21 . H213 . 109.5    no
C20 . C22 . H221 . 109.4    no
C20 . C22 . H222 . 109.5    no
H221 . C22 . H222 . 109.5    no
C20 . C22 . H223 . 109.5    no
H221 . C22 . H223 . 109.5    no
H222 . C22 . H223 . 109.5    no
C20 . C23 . H231 . 109.7    no
C20 . C23 . H232 . 109.6    no
H231 . C23 . H232 . 109.5    no
C20 . C23 . H233 . 109.1    no
H231 . C23 . H233 . 109.5    no
H232 . C23 . H233 . 109.5    no
C19 . C24 . H241 . 109.2    no
C19 . C24 . H242 . 109.5    no
H241 . C24 . H242 . 109.5    no
C19 . C24 . H243 . 109.7    no
H241 . C24 . H243 . 109.5    no
H242 . C24 . H243 . 109.5    no
O1 . C25 . C26 . 105.5(3)    yes
O1 . C25 . H251 . 110.1    no
C26 . C25 . H251 . 110.3    no
O1 . C25 . H252 . 110.9    no
C26 . C25 . H252 . 110.5    no
H251 . C25 . H252 . 109.5    no
C25 . C26 . C27 . 102.2(3)    yes
C25 . C26 . H261 . 111.3    no
C27 . C26 . H261 . 111.3    no
C25 . C26 . H262 . 111.4    no
C27 . C26 . H262 . 111.0    no
H261 . C26 . H262 . 109.5    no
C26 . C27 . C28 . 103.1(3)    yes
C26 . C27 . H271 . 111.1    no
C28 . C27 . H271 . 110.9    no
C26 . C27 . H272 . 111.2    no
C28 . C27 . H272 . 110.9    no
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H271 . C27 . H272 . 109.5    no
C27 . C28 . O1 . 105.9(3)    yes
C27 . C28 . H281 . 110.4    no
O1 . C28 . H281 . 109.7    no
C27 . C28 . H282 . 110.6    no
O1 . C28 . H282 . 110.7    no
H281 . C28 . H282 . 109.5    no
N2 . B1 . N4 . 112.1(3)    yes
N2 . B1 . N6 . 110.6(3)    yes
N4 . B1 . N6 . 110.0(3)    yes
N2 . B1 . H1 . 109(2)    no
N4 . B1 . H1 . 101(2)    no
N6 . B1 . H1 . 114(2)    no
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