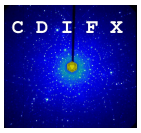

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CRYSCAL version : Sept. 2013 [T. Roisnel (CDIFX / ISCR UMR6226 - Rennes)]

PS143: Crystal structure report

X-ray crystallographic study

(C_{16} H_{16} N_4); $M = 264.33$. APEXII, Bruker-AXS diffractometer, $Mo - K_\alpha$ radiation (λ = 0.71073 Å), $T = 150(2)K$; triclinic $P\overline{1}$ (I.T.#2), $a = 5.8977(6), b = 7.4177(7), c = 30.865(3)$ Å, $\alpha; = 91.949(4), \beta; = 92.578(5), \gamma; = 94.343(4)$ °, $V = 1344.1(2)$ Å^3, $Z = 4$, $d = 1.306$ $g.cm^{-3}$, $\mu = 0.081$ mm^{-1}. The structure was solved by direct methods using the SIR97 program [1], and then refined with full-matrix least-square methods based on F^2 (SHELXL-97) [2] with the aid of the WINGX [3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 6089 unique intensities and 365 parameters converged at $\omega R(F^2) = 0.139$ ($RF = 0.0589$) for 4195 observed reflections with ($I > 2\sigma$).

1. A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, J. Appl. Cryst. (1999) 32, 115-119
2. Sheldrick G.M., Acta Cryst. A64 (2008), 112-122
3. L. J. Farrugia, J. Appl. Cryst., 2012, 45, 849-854

Structural data

Empirical formula	$C_{16}H_{16}N_4$
Formula weight	264.33
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, $P\ \overline{1}$
Unit cell dimensions	a = 5.8977(6) Å, α = 91.949(4) °
	b = 7.4177(7) Å, β = 92.578(5) °
	c = 30.865(3) Å, γ = 94.343(4) °
Volume	1344.1(2) Å^3
Z, Calculated density	4 , 1.306 ($g.cm^{-1}$)
Absorption coefficient	0.081 mm^{-1}
F(000)	560
Crystal size	0.6 x 0.47 x 0.07 mm
Crystal color	colourless
Theta range for data collection	3.01 to 27.44 °
h_min, h_max	-7 , 7
k_min, k_max	-9 , 9
l_min, l_max	-39 , 39
Reflections collected / unique	16133 / 6089 [^{a}R(int) = 0.0623]
Reflections [$I > 2\sigma$]	4195
Completeness to theta_max	0.988
Absorption correction type	multi-scan
Max. and min. transmission	0.994 , 0.726
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6089 / 0 / 365
^{b}Goodness-of-fit	1.029
Final R indices [$I > 2\sigma$]	$^cR_1$ = 0.0589, $^dwR_2$ = 0.139
R indices (all data)	$^cR_1$ = 0.0884, $^dwR_2$ = 0.1541
Largest diff. peak and hole	0.323 and -0.276 $\overline{e}$.Å^{-3}

$^aR_{int} = \frac{\sum |F_o^2 - \langle F_o^2 \rangle|}{\sum F_o^2}$

$^bS = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{n-p} \right\}^{1/2}$

$^cR_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}$

$^dwR_2 = \left\{ \frac{\sum [w(F_o^2 - F_c^2)^2]}{\sum [w(F_o^2)^2]} \right\}^{1/2}$

$w = 1./[\sigma(F_o^2) + (aP)^2 + bP]$ with $P = [2F_c^2 + Max(F_o^2, 0)]/3$

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters ($A^2 \times 10^3$). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.7757(3)	0.1927(3)	-0.02461(6)	1	0.0303(4)
H1	0.6284	0.1374	-0.0202	1	0.036
C2	0.8367(3)	0.2398(3)	-0.06580(6)	1	0.0355(5)
H2	0.7296	0.2185	-0.0897	1	0.043
C3	1.0530(4)	0.3179(3)	-0.07237(6)	1	0.0366(5)
H3	1.0938	0.3501	-0.1007	1	0.044
C4	1.2090(3)	0.3486(3)	-0.03764(7)	1	0.0349(5)
H4	1.3576	0.4012	-0.0422	1	0.042
C5	1.1501(3)	0.3034(3)	0.00388(6)	1	0.0307(4)
H5	1.2575	0.3242	0.0277	1	0.037
C6	0.9324(3)	0.2273(2)	0.01006(6)	1	0.0252(4)
N7	0.8673(2)	0.1835(2)	0.05287(5)	1	0.0251(3)
N8	0.6434(3)	0.1563(2)	0.06108(5)	1	0.0328(4)
N9	0.6320(3)	0.1171(2)	0.10239(5)	1	0.0323(4)
C10	0.8484(3)	0.1203(2)	0.12086(6)	1	0.0242(4)
C11	0.9989(3)	0.1633(2)	0.08935(6)	1	0.0261(4)
H11	1.1603	0.1761	0.0924	1	0.031
C12	0.8916(3)	0.0793(2)	0.16650(6)	1	0.0237(4)
C13	0.7232(3)	-0.0065(2)	0.19056(6)	1	0.0261(4)
H13	0.5775	-0.0393	0.177	1	0.031
C14	0.7626(3)	-0.0452(3)	0.23379(6)	1	0.0277(4)
H14	0.6433	-0.1033	0.2491	1	0.033
C15	0.9750(3)	-0.0001(2)	0.25534(6)	1	0.0246(4)
C16	1.1447(3)	0.0871(3)	0.23113(6)	1	0.0295(4)
H16	1.2905	0.1209	0.2446	1	0.035
C17	1.1023(3)	0.1246(3)	0.18795(6)	1	0.0300(4)
H17	1.2207	0.183	0.1725	1	0.036
N18	1.0180(3)	-0.0441(2)	0.29802(5)	1	0.0340(4)
C19	0.8352(3)	-0.1106(3)	0.32414(6)	1	0.0367(5)
H19A	0.7401	-0.0118	0.3311	1	0.055
H19B	0.8988	-0.1571	0.351	1	0.055
H19C	0.7425	-0.2079	0.308	1	0.055
C20	1.2230(3)	0.0254(3)	0.32158(7)	1	0.0395(5)
H20A	1.3537	0.0104	0.3036	1	0.059
H20B	1.2416	-0.0408	0.3483	1	0.059
H20C	1.2139	0.1542	0.3289	1	0.059
C21	0.3699(3)	0.2054(2)	0.49817(6)	1	0.0273(4)
H21	0.2537	0.1918	0.4757	1	0.033
C22	0.3250(3)	0.1566(3)	0.54023(6)	1	0.0325(5)
H22	0.1767	0.1089	0.5466	1	0.039
C23	0.4950(3)	0.1769(3)	0.57295(6)	1	0.0341(5)
H23	0.4634	0.1419	0.6015	1	0.041
C24	0.7104(3)	0.2480(3)	0.56394(6)	1	0.0330(5)
H24	0.8264	0.2622	0.5864	1	0.04
C25	0.7585(3)	0.2990(3)	0.52215(6)	1	0.0280(4)
H25	0.9059	0.3497	0.516	1	0.034
C26	0.5887(3)	0.2748(2)	0.48971(5)	1	0.0228(4)
N27	0.6414(2)	0.3195(2)	0.44619(5)	1	0.0238(3)
N28	0.8610(3)	0.3281(2)	0.43454(5)	1	0.0325(4)
N29	0.8601(3)	0.3686(2)	0.39333(5)	1	0.0318(4)
C30	0.6413(3)	0.3849(2)	0.37823(6)	1	0.0229(4)
C31	0.4996(3)	0.3520(2)	0.41204(5)	1	0.0234(4)
H31	0.3384	0.3521	0.4115	1	0.028
C32	0.5837(3)	0.4313(2)	0.33338(5)	1	0.0228(4)
C33	0.7279(3)	0.3943(2)	0.30004(6)	1	0.0246(4)
H33	0.8661	0.341	0.3067	1	0.03
C34	0.6731(3)	0.4339(2)	0.25736(6)	1	0.0252(4)

H34	0.7747	0.4073	0.2354	1	0.03
C35	0.4706(3)	0.5124(2)	0.24598(5)	1	0.0226(4)
C36	0.3259(3)	0.5510(2)	0.27979(6)	1	0.0255(4)
H36	0.1883	0.6058	0.2734	1	0.031
C37	0.3826(3)	0.5099(2)	0.32220(6)	1	0.0254(4)
H37	0.2816	0.5359	0.3443	1	0.03
N38	0.4147(3)	0.5512(2)	0.20346(5)	1	0.0306(4)
C39	0.5673(3)	0.5147(3)	0.16927(6)	1	0.0351(5)
H39A	0.71	0.5907	0.1743	1	0.053
H39B	0.496	0.5418	0.1412	1	0.053
H39C	0.5993	0.387	0.1692	1	0.053
C40	0.1986(3)	0.6154(3)	0.19099(6)	1	0.0359(5)
H40A	0.0761	0.5294	0.1997	1	0.054
H40B	0.1876	0.627	0.1594	1	0.054
H40C	0.1846	0.7337	0.2053	1	0.054

Anisotropic displacement parameters (Å^2)

The anisotropic displacement factor exponent takes the form: $-2\pi[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Atom	U11	U22	U33	U23	U13	U12
C1	0.0284(10)	0.0308(11)	0.0313(10)	0.0016(8)	-0.0001(8)	0.0010(8)
C2	0.0380(12)	0.0389(12)	0.0296(10)	0.0009(9)	-0.0029(9)	0.0051(9)
C3	0.0421(13)	0.0394(12)	0.0303(11)	0.0072(9)	0.0069(9)	0.0099(9)
C4	0.0293(11)	0.0362(12)	0.0409(11)	0.0106(9)	0.0070(9)	0.0066(9)
C5	0.0252(10)	0.0317(11)	0.0357(11)	0.0046(8)	-0.0016(8)	0.0044(8)
C6	0.0263(10)	0.0223(10)	0.0277(9)	0.0023(7)	0.0017(7)	0.0065(7)
N7	0.0202(8)	0.0265(8)	0.0284(8)	0.0019(6)	-0.0009(6)	0.0021(6)
N8	0.0225(9)	0.0441(10)	0.0315(9)	0.0020(7)	0.0010(7)	0.0019(7)
N9	0.0251(9)	0.0441(10)	0.0273(8)	0.0025(7)	-0.0018(7)	0.0014(7)
C10	0.0219(9)	0.0223(10)	0.0279(9)	-0.0025(7)	0.0002(7)	0.0014(7)
C11	0.0215(9)	0.0259(10)	0.0307(10)	0.0025(8)	-0.0014(7)	0.0017(7)
C12	0.0226(9)	0.0216(9)	0.0272(9)	-0.0006(7)	0.0005(7)	0.0037(7)
C13	0.0196(9)	0.0286(10)	0.0290(9)	-0.0023(8)	-0.0020(7)	-0.0028(7)
C14	0.0218(10)	0.0294(10)	0.0313(10)	0.0036(8)	0.0025(7)	-0.0035(7)
C15	0.0245(9)	0.0199(9)	0.0299(9)	0.0029(7)	0.0002(7)	0.0050(7)
C16	0.0201(10)	0.0308(11)	0.0363(11)	0.0041(8)	-0.0055(8)	-0.0034(8)
C17	0.0214(10)	0.0321(11)	0.0361(10)	0.0084(8)	0.0012(8)	-0.0041(8)
N18	0.0234(9)	0.0468(11)	0.0313(9)	0.0094(8)	-0.0016(7)	-0.0012(7)
C19	0.0305(11)	0.0455(13)	0.0333(11)	0.0114(9)	-0.0024(8)	-0.0050(9)
C20	0.0332(12)	0.0464(13)	0.0369(11)	0.0124(10)	-0.0099(9)	-0.0079(9)
C21	0.0249(10)	0.0302(10)	0.0275(9)	0.0049(8)	-0.0003(7)	0.0050(8)
C22	0.0292(11)	0.0354(12)	0.0351(11)	0.0106(9)	0.0085(8)	0.0093(8)
C23	0.0405(12)	0.0414(12)	0.0229(9)	0.0066(8)	0.0055(8)	0.0141(9)
C24	0.0363(12)	0.0398(12)	0.0239(10)	0.0008(8)	-0.0026(8)	0.0113(9)
C25	0.0259(10)	0.0296(10)	0.0286(10)	0.0023(8)	-0.0012(8)	0.0036(8)
C26	0.0252(9)	0.0226(9)	0.0214(9)	0.0029(7)	0.0004(7)	0.0060(7)
N27	0.0192(8)	0.0275(8)	0.0247(8)	0.0034(6)	-0.0011(6)	0.0012(6)
N28	0.0209(8)	0.0496(11)	0.0271(8)	0.0071(7)	-0.0001(6)	0.0016(7)
N29	0.0234(9)	0.0453(11)	0.0266(8)	0.0065(7)	-0.0009(6)	0.0012(7)
C30	0.0199(9)	0.0220(9)	0.0267(9)	0.0025(7)	-0.0006(7)	0.0009(7)
C31	0.0205(9)	0.0245(10)	0.0251(9)	0.0034(7)	-0.0017(7)	0.0022(7)
C32	0.0210(9)	0.0224(9)	0.0245(9)	0.0038(7)	-0.0014(7)	-0.0014(7)
C33	0.0191(9)	0.0247(10)	0.0303(10)	0.0038(8)	0.0003(7)	0.0024(7)
C34	0.0234(10)	0.0275(10)	0.0246(9)	0.0009(7)	0.0041(7)	-0.0001(7)
C35	0.0205(9)	0.0229(9)	0.0237(9)	0.0020(7)	-0.0014(7)	-0.0028(7)
C36	0.0199(9)	0.0286(10)	0.0279(9)	0.0020(8)	-0.0009(7)	0.0028(7)
C37	0.0234(9)	0.0270(10)	0.0261(9)	0.0004(7)	0.0041(7)	0.0020(7)
N38	0.0215(8)	0.0483(11)	0.0219(8)	0.0038(7)	-0.0010(6)	0.0023(7)
C39	0.0304(11)	0.0511(14)	0.0246(10)	0.0042(9)	0.0025(8)	0.0058(9)
C40	0.0325(11)	0.0461(13)	0.0308(10)	0.0090(9)	0.0015(8)	0.0105(9)

Bond length [Å]

```
C1   - C2       = 1.385(3)
C1   - C6       = 1.386(3)
C1   - H1       = 0.95
C2   - C3       = 1.387(3)
C2   - H2       = 0.95
C3   - C4       = 1.382(3)
C3   - H3       = 0.95
C4   - C5       = 1.388(3)
C4   - H4       = 0.95
C5   - C6       = 1.386(3)
C5   - H5       = 0.95
C6   - N7       = 1.433(2)
N7   - N8       = 1.357(2)
N7   - C11      = 1.357(2)
N8   - N9       = 1.321(2)
N9   - C10      = 1.373(2)
C10  - C11      = 1.375(2)
C10  - C12      = 1.466(2)
C11  - H11      = 0.95
C12  - C17      = 1.394(2)
C12  - C13      = 1.395(2)
C13  - C14      = 1.387(2)
C13  - H13      = 0.95
C14  - C15      = 1.404(2)
C14  - H14      = 0.95
C15  - N18      = 1.385(2)
C15  - C16      = 1.407(2)
C16  - C17      = 1.386(2)
C16  - H16      = 0.95
C17  - H17      = 0.95
N18  - C20      = 1.435(2)
N18  - C19      = 1.442(2)
C19  - H19A     = 0.98
C19  - H19B     = 0.98
C19  - H19C     = 0.98
C20  - H20A     = 0.98
C20  - H20B     = 0.98
C20  - H20C     = 0.98
C21  - C22      = 1.391(2)
C21  - C26      = 1.392(3)
C21  - H21      = 0.95
C22  - C23      = 1.387(3)
C22  - H22      = 0.95
C23  - C24      = 1.382(3)
C23  - H23      = 0.95
C24  - C25      = 1.392(2)
C24  - H24      = 0.95
C25  - C26      = 1.381(2)
C25  - H25      = 0.95
C26  - N27      = 1.436(2)
N27  - C31      = 1.355(2)
N27  - N28      = 1.357(2)
N28  - N29      = 1.317(2)
N29  - C30      = 1.368(2)
C30  - C31      = 1.383(2)
C30  - C32      = 1.469(2)
C31  - H31      = 0.95
C32  - C37      = 1.396(2)
C32  - C33      = 1.397(2)
C33  - C34      = 1.389(2)
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C33  - H33      = 0.95
C34  - C35      = 1.404(2)
C34  - H34      = 0.95
C35  - N38      = 1.384(2)
C35  - C36      = 1.413(2)
C36  - C37      = 1.386(2)
C36  - H36      = 0.95
C37  - H37      = 0.95
N38  - C40      = 1.435(2)
N38  - C39      = 1.449(2)
C39  - H39A     = 0.98
C39  - H39B     = 0.98
C39  - H39C     = 0.98
C40  - H40A     = 0.98
C40  - H40B     = 0.98
C40  - H40C     = 0.98
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Angles [°]

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C2      - C1      - C6      = 119.18(18)
C2      - C1      - H1      = 120.4
C6      - C1      - H1      = 120.4
C1      - C2      - C3      = 120.41(18)
C1      - C2      - H2      = 119.8
C3      - C2      - H2      = 119.8
C4      - C3      - C2      = 119.82(18)
C4      - C3      - H3      = 120.1
C2      - C3      - H3      = 120.1
C3      - C4      - C5      = 120.46(18)
C3      - C4      - H4      = 119.8
C5      - C4      - H4      = 119.8
C6      - C5      - C4      = 119.11(18)
C6      - C5      - H5      = 120.4
C4      - C5      - H5      = 120.4
C1      - C6      - C5      = 120.99(17)
C1      - C6      - N7      = 119.22(16)
C5      - C6      - N7      = 119.80(16)
N8      - N7      - C11     = 110.50(14)
N8      - N7      - C6      = 119.69(14)
C11     - N7      - C6      = 129.80(15)
N9      - N8      - N7      = 107.15(14)
N8      - N9      - C10     = 109.16(15)
N9      - C10     - C11     = 107.93(16)
N9      - C10     - C12     = 122.03(16)
C11     - C10     - C12     = 130.03(16)
N7      - C11     - C10     = 105.26(16)
N7      - C11     - H11     = 127.4
C10     - C11     - H11     = 127.4
C17     - C12     - C13     = 116.82(16)
C17     - C12     - C10     = 121.70(16)
C13     - C12     - C10     = 121.49(16)
C14     - C13     - C12     = 121.81(16)
C14     - C13     - H13     = 119.1
C12     - C13     - H13     = 119.1
C13     - C14     - C15     = 121.36(16)
C13     - C14     - H14     = 119.3
C15     - C14     - H14     = 119.3
N18     - C15     - C14     = 121.65(16)
N18     - C15     - C16     = 121.48(16)
C14     - C15     - C16     = 116.84(16)
C17     - C16     - C15     = 120.99(17)
C17     - C16     - H16     = 119.5
C15     - C16     - H16     = 119.5
C16     - C17     - C12     = 122.18(17)
C16     - C17     - H17     = 118.9
C12     - C17     - H17     = 118.9
C15     - N18     - C20     = 120.93(15)
C15     - N18     - C19     = 120.66(15)
C20     - N18     - C19     = 115.62(16)
N18     - C19     - H19A    = 109.5
N18     - C19     - H19B    = 109.5
H19A    - C19     - H19B    = 109.5
N18     - C19     - H19C    = 109.5
H19A    - C19     - H19C    = 109.5
H19B    - C19     - H19C    = 109.5
N18     - C20     - H20A    = 109.5
N18     - C20     - H20B    = 109.5
H20A    - C20     - H20B    = 109.5
N18     - C20     - H20C    = 109.5
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H20A     - C20      - H20C     = 109.5
H20B     - C20      - H20C     = 109.5
C22      - C21      - C26      = 118.55(17)
C22      - C21      - H21      = 120.7
C26      - C21      - H21      = 120.7
C23      - C22      - C21      = 120.57(18)
C23      - C22      - H22      = 119.7
C21      - C22      - H22      = 119.7
C24      - C23      - C22      = 119.90(17)
C24      - C23      - H23      = 120.1
C22      - C23      - H23      = 120.1
C23      - C24      - C25      = 120.47(18)
C23      - C24      - H24      = 119.8
C25      - C24      - H24      = 119.8
C26      - C25      - C24      = 119.01(17)
C26      - C25      - H25      = 120.5
C24      - C25      - H25      = 120.5
C25      - C26      - C21      = 121.48(16)
C25      - C26      - N27      = 118.96(16)
C21      - C26      - N27      = 119.54(15)
C31      - N27      - N28      = 110.88(14)
C31      - N27      - C26      = 129.49(15)
N28      - N27      - C26      = 119.60(14)
N29      - N28      - N27      = 106.94(14)
N28      - N29      - C30      = 109.50(15)
N29      - C30      - C31      = 107.90(15)
N29      - C30      - C32      = 122.71(16)
C31      - C30      - C32      = 129.39(16)
N27      - C31      - C30      = 104.76(15)
N27      - C31      - H31      = 127.6
C30      - C31      - H31      = 127.6
C37      - C32      - C33      = 117.50(16)
C37      - C32      - C30      = 121.77(16)
C33      - C32      - C30      = 120.72(16)
C34      - C33      - C32      = 121.30(16)
C34      - C33      - H33      = 119.3
C32      - C33      - H33      = 119.3
C33      - C34      - C35      = 121.35(16)
C33      - C34      - H34      = 119.3
C35      - C34      - H34      = 119.3
N38      - C35      - C34      = 121.54(16)
N38      - C35      - C36      = 121.19(16)
C34      - C35      - C36      = 117.27(15)
C37      - C36      - C35      = 120.65(17)
C37      - C36      - H36      = 119.7
C35      - C36      - H36      = 119.7
C36      - C37      - C32      = 121.93(16)
C36      - C37      - H37      = 119
C32      - C37      - H37      = 119
C35      - N38      - C40      = 121.77(15)
C35      - N38      - C39      = 120.56(16)
C40      - N38      - C39      = 117.51(15)
N38      - C39      - H39A     = 109.5
N38      - C39      - H39B     = 109.5
H39A     - C39      - H39B     = 109.5
N38      - C39      - H39C     = 109.5
H39A     - C39      - H39C     = 109.5
H39B     - C39      - H39C     = 109.5
N38      - C40      - H40A     = 109.5
N38      - C40      - H40B     = 109.5
H40A     - C40      - H40B     = 109.5
N38      - C40      - H40C     = 109.5
H40A     - C40      - H40C     = 109.5
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H40B      - C40       - H40C      = 109.5
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Torsion angles [°]

C6	- C1	- C2	- C3	= 1.0(3)
C1	- C2	- C3	- C4	= 0.1(3)
C2	- C3	- C4	- C5	= -0.5(3)
C3	- C4	- C5	- C6	= -0.2(3)
C2	- C1	- C6	- C5	= -1.8(3)
C2	- C1	- C6	- N7	= 178.19(16)
C4	- C5	- C6	- C1	= 1.3(3)
C4	- C5	- C6	- N7	= -178.62(16)
C1	- C6	- N7	- N8	= -17.8(3)
C5	- C6	- N7	- N8	= 162.15(17)
C1	- C6	- N7	- C11	= 162.39(18)
C5	- C6	- N7	- C11	= -17.6(3)
C11	- N7	- N8	- N9	= -0.6(2)
C6	- N7	- N8	- N9	= 179.54(15)
N7	- N8	- N9	- C10	= 0.4(2)
N8	- N9	- C10	- C11	= 0.0(2)
N8	- N9	- C10	- C12	= -179.02(16)
N8	- N7	- C11	- C10	= 0.6(2)
C6	- N7	- C11	- C10	= -179.59(17)
N9	- C10	- C11	- N7	= -0.4(2)
C12	- C10	- C11	- N7	= 178.54(17)
N9	- C10	- C12	- C17	= -164.02(18)
C11	- C10	- C12	- C17	= 17.2(3)
N9	- C10	- C12	- C13	= 15.8(3)
C11	- C10	- C12	- C13	= -162.98(19)
C17	- C12	- C13	- C14	= 0.0(3)
C10	- C12	- C13	- C14	= -179.79(17)
C12	- C13	- C14	- C15	= -0.2(3)
C13	- C14	- C15	- N18	= -177.65(17)
C13	- C14	- C15	- C16	= 0.5(3)
N18	- C15	- C16	- C17	= 177.61(17)
C14	- C15	- C16	- C17	= -0.6(3)
C15	- C16	- C17	- C12	= 0.3(3)
C13	- C12	- C17	- C16	= -0.1(3)
C10	- C12	- C17	- C16	= 179.74(17)
C14	- C15	- N18	- C20	= -170.75(19)
C16	- C15	- N18	- C20	= 11.2(3)
C14	- C15	- N18	- C19	= -10.5(3)
C16	- C15	- N18	- C19	= 171.42(18)
C26	- C21	- C22	- C23	= 0.1(3)
C21	- C22	- C23	- C24	= 0.7(3)
C22	- C23	- C24	- C25	= -0.2(3)
C23	- C24	- C25	- C26	= -1.0(3)
C24	- C25	- C26	- C21	= 1.8(3)
C24	- C25	- C26	- N27	= -177.09(16)
C22	- C21	- C26	- C25	= -1.3(3)
C22	- C21	- C26	- N27	= 177.54(16)
C25	- C26	- N27	- C31	= -161.22(18)
C21	- C26	- N27	- C31	= 19.9(3)
C25	- C26	- N27	- N28	= 21.0(2)
C21	- C26	- N27	- N28	= -157.94(17)
C31	- N27	- N28	- N29	= 1.0(2)
C26	- N27	- N28	- N29	= 179.16(15)
N27	- N28	- N29	- C30	= -0.4(2)
N28	- N29	- C30	- C31	= -0.2(2)
N28	- N29	- C30	- C32	= 179.39(16)
N28	- N27	- C31	- C30	= -1.06(19)
C26	- N27	- C31	- C30	= -179.03(16)
N29	- C30	- C31	- N27	= 0.76(19)
C32	- C30	- C31	- N27	= -178.80(17)

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N29      - C30      - C32      - C37      = -156.56(18)
C31      - C30      - C32      - C37      = 22.9(3)
N29      - C30      - C32      - C33      = 24.8(3)
C31      - C30      - C32      - C33      = -155.73(18)
C37      - C32      - C33      - C34      = -0.1(3)
C30      - C32      - C33      - C34      = 178.61(16)
C32      - C33      - C34      - C35      = -0.1(3)
C33      - C34      - C35      - N38      = -179.66(16)
C33      - C34      - C35      - C36      = 0.6(3)
N38      - C35      - C36      - C37      = 179.36(16)
C34      - C35      - C36      - C37      = -0.9(2)
C35      - C36      - C37      - C32      = 0.7(3)
C33      - C32      - C37      - C36      = -0.2(3)
C30      - C32      - C37      - C36      = -178.91(16)
C34      - C35      - N38      - C40      = 173.99(17)
C36      - C35      - N38      - C40      = -6.3(3)
C34      - C35      - N38      - C39      = -1.2(3)
C36      - C35      - N38      - C39      = 178.55(17)
```
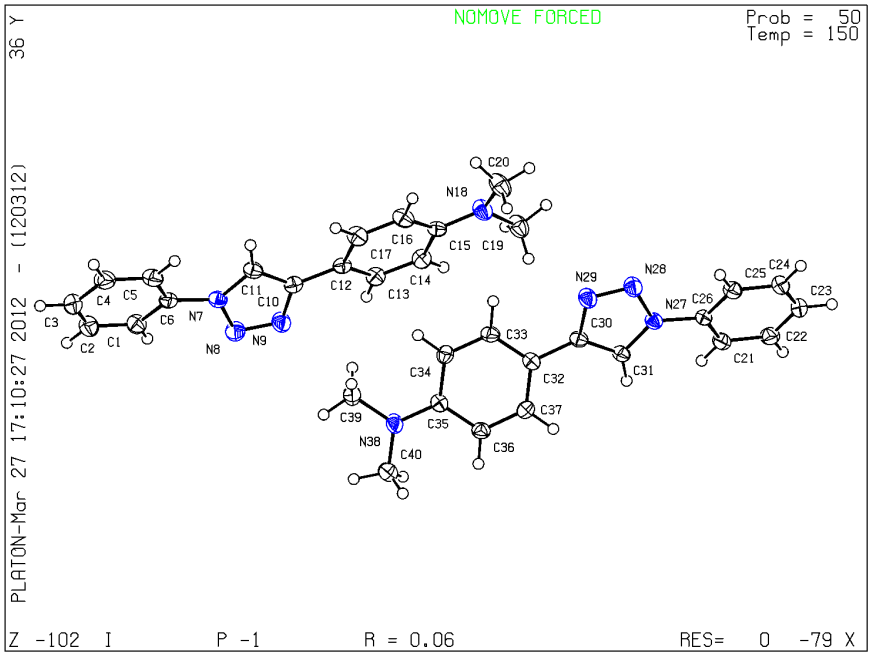

Structure visualisation



This structural report has been created through CRYSCAL (Sept. 2013). Please report bugs and problems to cdifx@univ-rennes1.fr