checkCIF/PLATON report (basic structural check)

No syntax errors found.
Please wait while processing ....

CIF dictionary
Interpreting this report

Datablock: Compound2d

Bond precision: C-C = 0.0016 A Wavelength=0.71073

Cell: a=11.8968(3) b=7.4738(2) c=24.2583(7)
alpha=90 beta=97.199(1) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	2139.91(10)	2139.91(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H37 Al2 Nd	C17 H37 Al2 Nd
Sum formula	C17 H37 Al2 Nd	C17 H37 Al2 Nd
Mr	439.67	439.67
Dx,g cm-3	1.365	1.365
Z	4	4
Mu (mm-1)	2.500	2.500
F000	900.0	900.0
F000'	899.86	
h,k,lmax	16,10,34	16,10,34
Nref	6321	6307
Tmin,Tmax	0.436,0.577	0.354,0.603
Tmin'	0.270	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 30.140

R(reflections)= 0.0137(6129) wR2(reflections)= 0.0354(6307)

S = 1.177 Npar= 241

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	63.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	141.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	131.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	139.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	63.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	131.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C4	X-C-H Bond Angle	125.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	172.20 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	72.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	82.00 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	92.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	126.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	72.70 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	171.90 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	82.50 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	127.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	92.30 Deg.

Alert level B

PLAT390_ALERT_3_B Deviating Methyl C1 X-C-H Bond Angle ..... 95.10 Deg.
PLAT390_ALERT_3_B Deviating Methyl C2 X-C-H Bond Angle ..... 96.20 Deg.

Alert level C

PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.94 Ratio
PLAT390_ALERT_3_C Deviating Methyl C5 X-C-H Bond Angle ..... 117.80 Deg.
PLAT390_ALERT_3_C Deviating Methyl C6 X-C-H Bond Angle ..... 116.60 Deg.

Alert level G

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 30
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 16

17 **ALERT level A** = In general: serious problem
2 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
2 **ALERT level G** = General alerts; check

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 ALERT type 2 Indicator that the structure model may be wrong or deficient
23 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF in IUCr journals

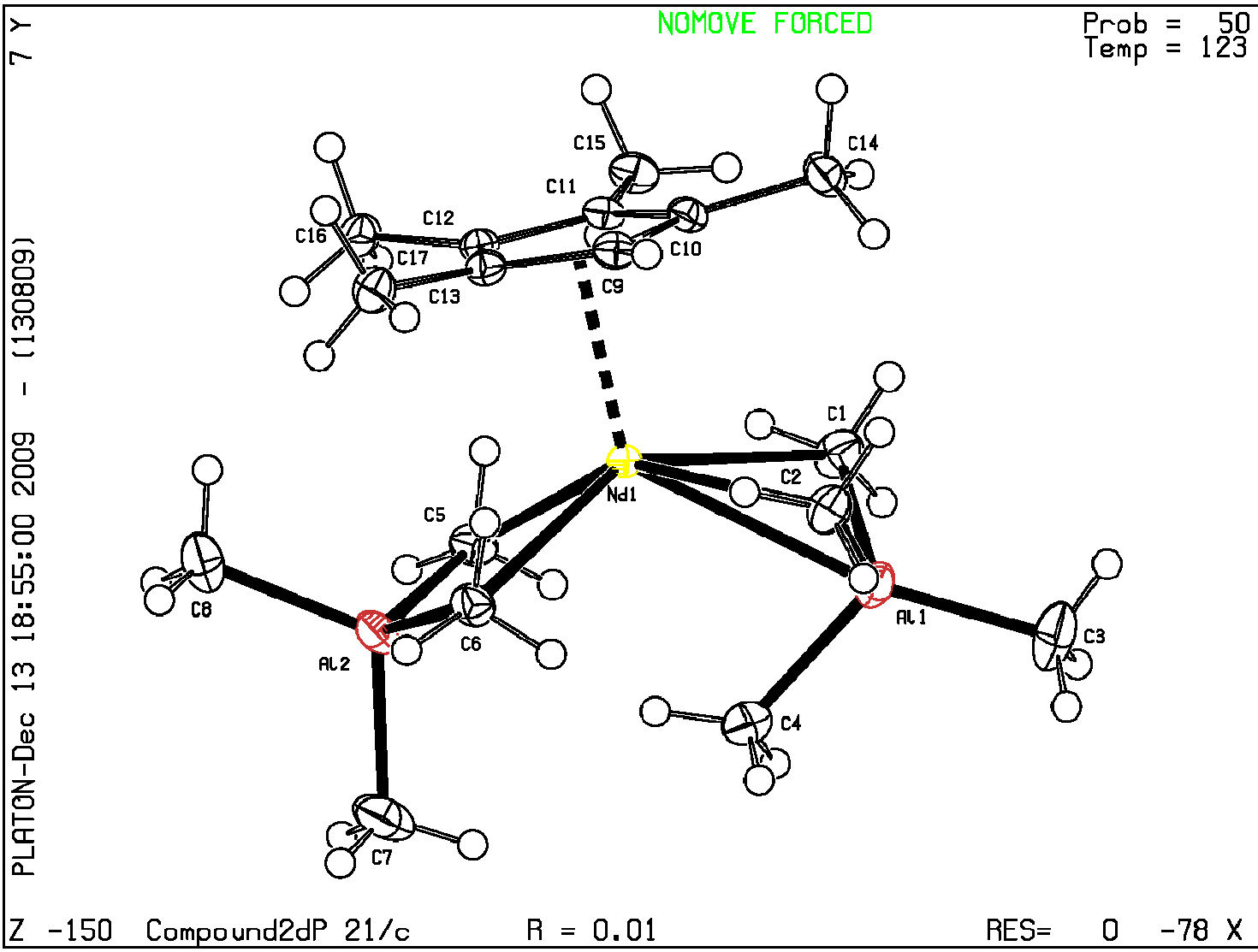
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publicatio IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); howe you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication checks are r the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 13/08/2009; check.def file version of 12/08/2009

Datablock Compound2d - ellipsoid plot



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