checkCIF/PLATON report (basic structural check)

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

CIF dictionary
Interpreting this report

Datablock: Compound2c

Bond precision: C-C = 0.0019 A Wavelength=0.71073

Cell: a=11.8277(4) b=7.4655(3) c=24.1851(9)
alpha=90 beta=97.166(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2118.86(14)	2118.86(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C17 H37 Al2 Sm	C17 H37 Al2 Sm
Sum formula	C17 H37 Al2 Sm	C17 H37 Al2 Sm
Mr	445.79	445.78
Dx,g cm-3	1.398	1.397
Z	4	4
Mu (mm-1)	2.846	2.846
F000	908.0	908.0
F000'	907.99	
h,k,lmax	16,10,34	16,10,34
Nref	6242	6225
Tmin,Tmax	0.315,0.796	0.378,0.815
Tmin'	0.283	

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 30.110

R(reflections)= 0.0165(6015) wR2(reflections)= 0.0407(6225)

S = 1.192 Npar= 242

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	64.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	138.50 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	133.20 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	93.20 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	137.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	64.70 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	94.70 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	133.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C4	X-C-H Bond Angle	125.20 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	169.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	72.70 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	84.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	91.20 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	127.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	73.70 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	170.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	84.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	128.80 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	89.90 Deg.

Alert level B

PLAT222_ALERT_3_B Large Non-Solvent H Ueq(max)/Ueq(min) ... 4.25 Ratio

Alert level C

PLAT390_ALERT_3_C Deviating Methyl C5 X-C-H Bond Angle ..... 117.30 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

19 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
2 **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

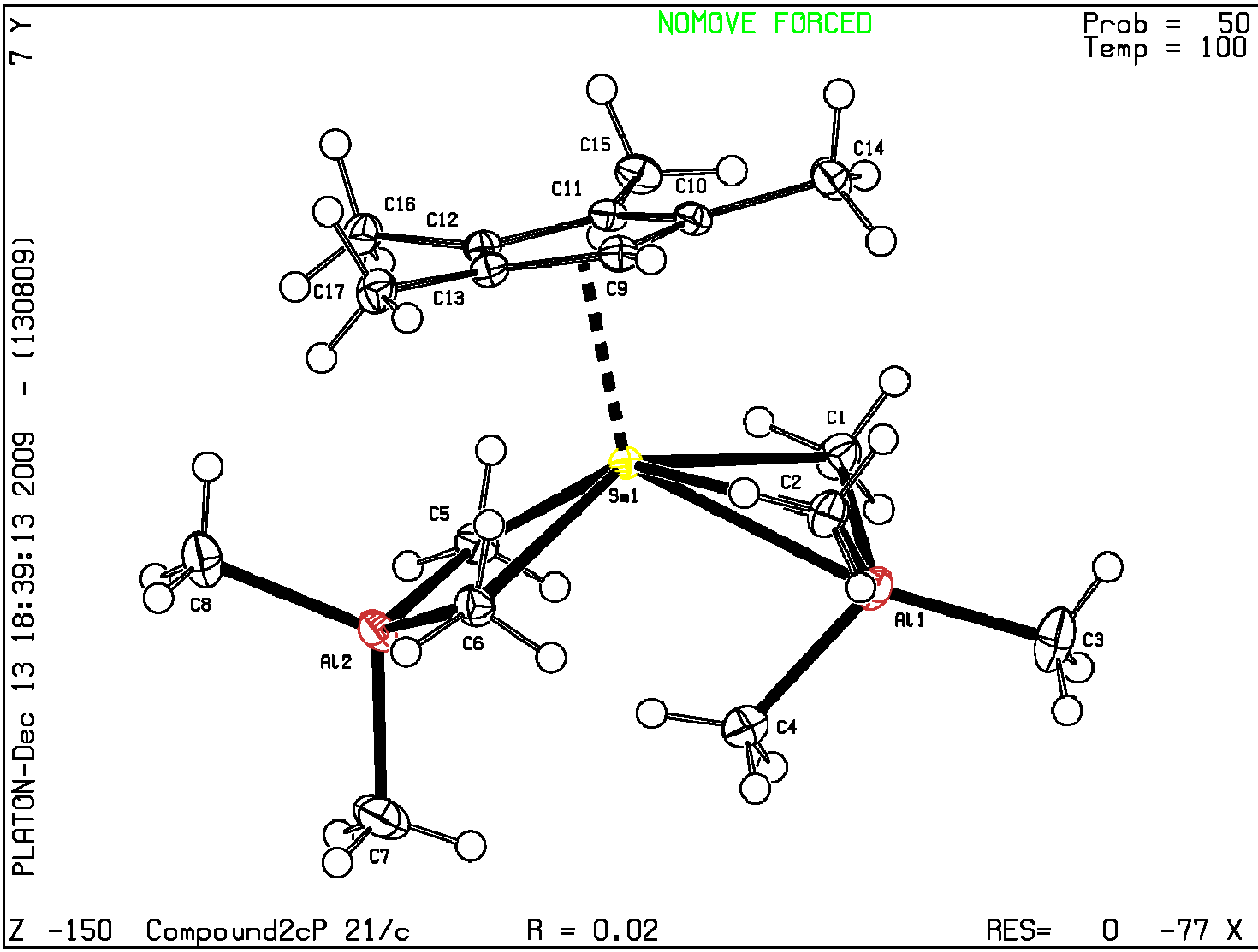
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publicatio IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); howe you intend to submit to *Acta Crystallographica Section C* or *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 Compound2c - ellipsoid plot



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