

checkCIF/PLATON report (basic structural check)

No syntax errors found.

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[Interpreting this report](#)

Datablock: Compound2e

Bond precision: C-C = 0.0018 Å Wavelength=0.71073

Cell: a=10.4725(8) b=10.7491(8) c=11.9506(9)
alpha=74.043(1) beta=66.316(1) gamma=63.932(1)

Temperature: 123 K

	Calculated	Reported
Volume	1098.70(14)	1098.70(14)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C34 H74 Al4 La2	C34 H74 Al4 La2
Sum formula	C34 H74 Al4 La2	C34 H74 Al4 La2
Mr	868.67	868.67
Dx, g cm ⁻³	1.313	1.313
Z	1	1
Mu (mm ⁻¹)	2.016	2.016
F000	444.0	444.0
F000'	443.74	
h, k, lmax	14, 15, 16	14, 15, 16
Nref	6485	6470
Tmin, Tmax	0.526, 0.629	0.368, 0.654
Tmin'	0.347	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 30.110

R(reflections)= 0.0126(6330) wR2(reflections)= 0.0333(6470)

S = 1.120 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	174.10 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	72.50 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C1	X-C-H Bond Angle	73.00 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C2	X-C-H Bond Angle	94.30 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	71.50 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	84.00 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	171.90 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	126.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C5	X-C-H Bond Angle	94.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	73.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	81.90 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	170.40 Deg.
PLAT390_ALERT_3_A	Deviating Methyl C6	X-C-H Bond Angle	88.40 Deg.
PLAT780_ALERT_1_A	Coordinates do not Form a Properly Connected Set			?

Alert level B

PLAT390_ALERT_3_B	Deviating Methyl C1	X-C-H Bond Angle	97.20 Deg.
PLAT390_ALERT_3_B	Deviating Methyl C1	X-C-H Bond Angle	119.80 Deg.
PLAT390_ALERT_3_B	Deviating Methyl C1	X-C-H Bond Angle	120.60 Deg.

PLAT390_ALERT_3_B	Deviating Methyl C2	X-C-H Bond Angle	121.20 Deg.
PLAT390_ALERT_3_B	Deviating Methyl C2	X-C-H Bond Angle	119.60 Deg.
PLAT390_ALERT_3_B	Deviating Methyl C6	X-C-H Bond Angle	123.50 Deg.
PLAT390_ALERT_3_B	Deviating Methyl C6	X-C-H Bond Angle	120.00 Deg.

● Alert level C

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.26	
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Al2 -- C8 ..	5.10 su	
PLAT390_ALERT_3_C	Deviating Methyl C5	X-C-H Bond Angle	116.50 Deg.

● Alert level G

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	30
PLAT154_ALERT_1_G	The su's on the Cell Angles are Equal (x 10000)	100 Deg.
PLAT164_ALERT_4_G	Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.	16
PLAT764_ALERT_4_G	Overcomplete CIF Bond List Detected (Rep/Expd) .	1.28 Ratio

- 14 **ALERT level A** = In general: serious problem
7 **ALERT level B** = Potentially serious problem
3 **ALERT level C** = Check and explain
4 **ALERT level G** = General alerts; check
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
22 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Publication of your CIF in IUCr journals

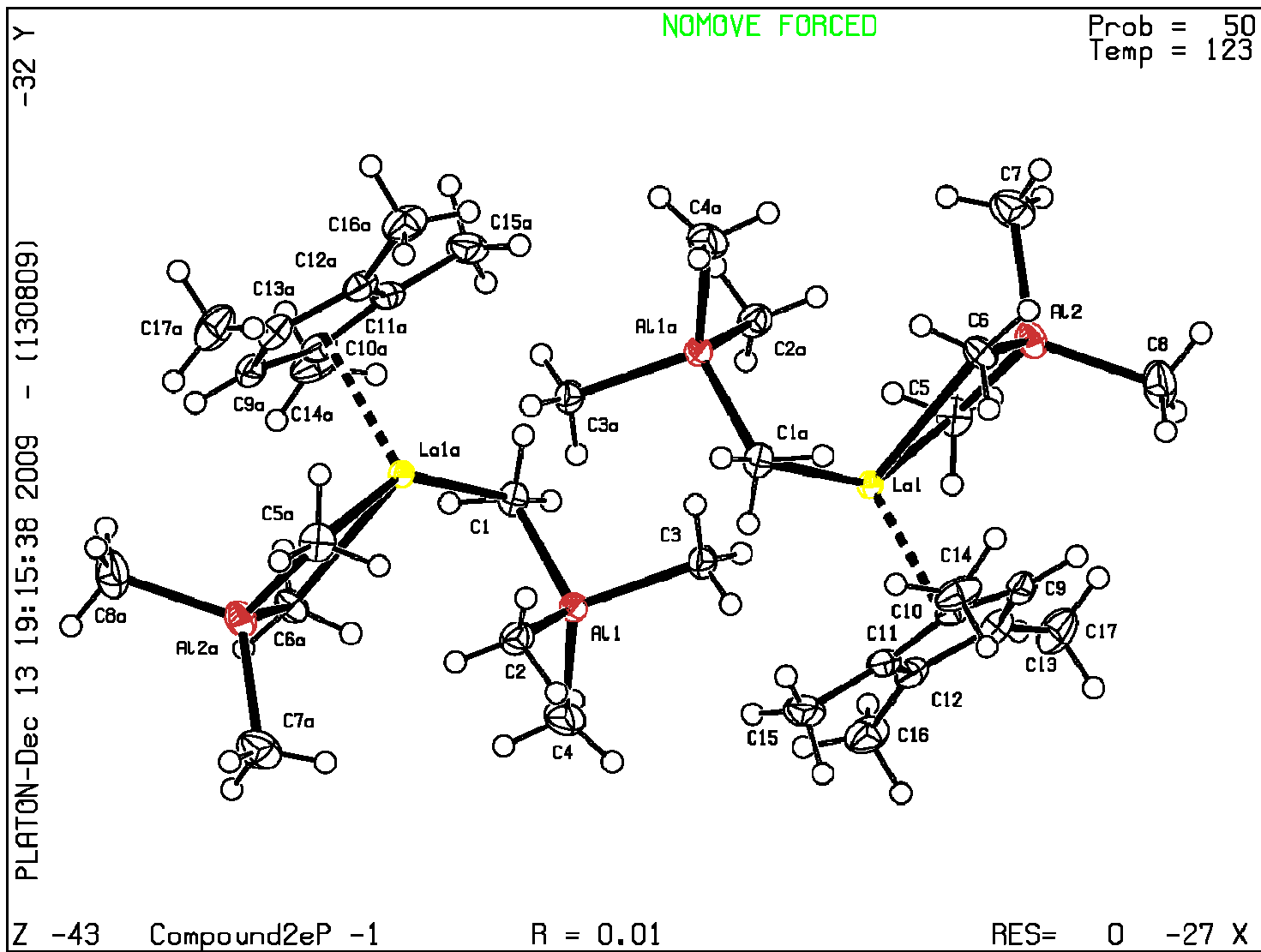
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that [full publication checks](#) are run on 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 Compound2e - ellipsoid plot



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