checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Sm

Bond precision: C-C = 0.0210 A Wavelength=0.71073

Cell: a=12.5315(10) b=19.113(2) c=19.993(2)
alpha=90 beta=98.934(8) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	4730.5(8)	4730.6(8)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C59 H45 N2 O6 Sm	Sm (C14 H12 N2) (C15 H11 O2)3
Sum formula	C59 H45 N2 O6 Sm	C59 H45 N2 O6 Sm
Mr	1028.33	1028.63
Dx,g cm-3	1.444	1.446
Z	4	4
Mu (mm-1)	1.297	1.297
F000	2092.0	2092.0
F000’	2092.12	
h,k,lmax	14,22,23	14,22,23
Nref	8457	8385
Tmin,Tmax	0.633,0.772	0.422,0.656
Tmin’	0.518	

Correction method= # Reported T Limits: Tmin=0.422 Tmax=0.656
AbsCorr = GAUSSIAN

Data completeness= 0.991 Theta(max)= 25.150

R(reflections)= 0.1177(6034) wR2(reflections)= 0.2285(8385)

S = 1.159 Npar= 615

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 B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0210 Ang.

Alert level C

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.118
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C19 has ADP max/min Ratio ..... 3.7 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.0 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference O4 -- C24 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C24 -- C25 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31 -- C37 .. 0.16 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C14 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C18 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C15 Check
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C1 - C7 ... 1.53 Ang.
PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C16 - C22 ... 1.54 Ang.

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C59 H45 N2 O6 Sm1
Atom count from _chemical_formula_moiety:
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 79.77 Why ?
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT982_ALERT_1_G The Sm-f'= -0.158 Deviates from the IT-value -0.164 Check
PLAT983_ALERT_1_G The Sm-f"= 3.668 Deviates from the IT-Value 3.442 Check

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

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

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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 21/04/2015; check.def file version of 09/03/2015

Datablock Sm - ellipsoid plot