

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 = 0.0067 A | Wavelength=0.71073 | |
| Cell: | a=19.1810(8) | b=20.1166(8) | c=24.1827(8) |
| | alpha=90 | beta=90 | gamma=90 |
| Temperature: | 100 K | | |
| | Calculated | Reported | |
| Volume | 9331.1(6) | 9331.1(6) | |
| Space group | P b c a | P b c a | |
| Hall group | -P 2ac 2ab | -P 2ac 2ab | |
| Moiety formula | C57 H45 N2 O6 Sm | Sm (C12 H12 N2) (C15 H11 O2)3 | |
| Sum formula | C57 H45 N2 O6 Sm | C57 H45 N2 O6 Sm | |
| Mr | 1004.31 | 1004.31 | |
| Dx,g cm-3 | 1.430 | 1.430 | |
| Z | 8 | 8 | |
| Mu (mm-1) | 1.313 | 1.313 | |
| F000 | 4088.0 | 4088.0 | |
| F000' | 4088.21 | | |
| h,k,lmax | 24,26,31 | 24,26,31 | |
| Nref | 10796 | 10767 | |
| Tmin,Tmax | 0.538,0.674 | 0.572,0.747 | |
| Tmin' | 0.514 | | |

Correction method= # Reported T Limits: Tmin=0.572 Tmax=0.747
AbsCorr = GAUSSIAN

Data completeness= 0.997 Theta(max)= 27.580

R(reflections)= 0.0427(7590) wR2(reflections)= 0.1131(10767)

S = 1.044 Npar= 597

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

PLAT230_ALERT_2_B Hirshfeld Test Diff for C54 -- C55 .. 7.2 su

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: C57 H45 N2 O6 Sml

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. | 14.61 Why ? |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Sml -- N1 .. | 5.5 su |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X) | Sml -- N2 .. | 5.9 su |
| PLAT899_ALERT_4_G | SHELXL97 | is Deprecated and Succeeded by SHELXL | 2014 Note |
| PLAT982_ALERT_1_G | The Sm-f'=' | -0.189 Deviates from the IT-value | -0.164 Check |
| PLAT983_ALERT_1_G | The Sm-f"=" | 4.410 Deviates from the IT-Value | 3.442 Check |

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

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

