# 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: sad

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Bond precision: C-C = 0.0183 A Wavelength=1.54178

Cell: a=16.5676(15) b=16.3937(14) c=16.2839(14)
alpha=90 beta=113.838(3) gamma=90
Temperature: 150 K

| | Calculated | Reported |
|---|---|---|
| Volume | 4045.5(6) | 4045.5(6) |
| Space group | C 2/c | C 1 2/c 1 |
| Hall group | -C 2yc | -C 2yc |
| Moiety formula | C36 H12 Eu2 O13 S12 [+ solvent] | C144 H48 Eu8 O52 S48 |
| Sum formula | C36 H12 Eu2 O13 S12 [+ solvent] | C144 H48 Eu8 O52 S48 |
| Mr | 1341.12 | 5364.38 |
| Dx,g cm-3 | 2.202 | 2.202 |
| Z | 4 | 1 |
| Mu (mm-1) | 28.361 | 28.361 |
| F000 | 2600.0 | 2600.0 |
| F000' | 2552.13 | |
| h,k,lmax | 19,19,19 | 19,19,19 |
| Nref | 3694 | 3655 |
| Tmin,Tmax | 0.063,0.059 | |
| Tmin' | 0.010 | |

Correction method= Not given

Data completeness= 0.989 Theta(max)= 68.237

R(reflections)= 0.0841( 3600) wR2(reflections)= 0.2168( 3655)

S = 1.083 Npar= 305

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 C**

```
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01829 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C13      - C15      .       1.54 Ang.
```

**Alert level G**

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         34 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......     Please Check
PLAT014_ALERT_1_G No       _shelx_fab_checksum Found in CIF ......     Please Check
PLAT042_ALERT_1_G Calc. and Reported Moiety Formula Strings Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...     4.0000 Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large     226.22 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          5 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          3 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records          3 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records          1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records          3 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O3       .        5.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O4_b     .       10.0 s.u.
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )         6% Note
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure         18 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Eu1       (III)     .       3.34 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        846 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
```

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

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

## Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT250_sad
;
PROBLEM: Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
RESPONSE: ...
```

```
;
_vrf_PLAT342_sad
;
PROBLEM: Low Bond Precision on  C-C Bonds ..............    0.01829 Ang.
RESPONSE: ...
;
_vrf_PLAT369_sad
;
PROBLEM: Long   C(sp2)-C(sp2) Bond  C13      - C15      .       1.54 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

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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* or *IUCrData*, 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.

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**PLATON version of 18/12/2021; check.def file version of 18/12/2021**

**Datablock sad** - ellipsoid plot