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: I

Bond precision: C-C = 0.0006 A Wavelength=1.54056

Cell: a=19.681(7) b=14.936(6) c=7.551(3)
alpha=90.931(19) beta=95.285(18) gamma=91.764(17)
Temperature: 293 K

	Calculated	Reported
Volume	2208.8(15)	2208.8(14)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C47 Eu O10	C47 Eu H35 O10
Sum formula	C47 Eu O10	C47 Eu H35 O10
Mr	876.44	876.47
Dx,g cm-3	0.659	0.659
Z	1	1
Mu (mm-1)	5.309	5.274
F000	425.0	0.0
F000'	417.51	
h,k,lmax	12,9,4	12,9,4
Nref	2524[1262]	1260
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 1.00/0.50 Theta(max)= 30.025

R(reflections)= wR2(reflections)=
S = Npar=

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

PLAT602_ALERT_2_A Solvent Accessible VOID(S) in the Unit-Cell .... ! Check

---

Alert level C

```
REFI015_ALERT_1_C  _refine_ls_shift/su_max is missing
           Maximum shift/s.u. ratio after final refinement cycle.
           The following tests will not be performed
           SHFSU_01
CHEMW01_ALERT_1_C  The ratio of given/expected molecular weight as calculated
           from the _chemical_formula_sum lies outside
           the range 0.99 <> 1.01
           Calculated formula weight =   911.7475
           Formula weight given      =   876.4670
CHEMW01_ALERT_1_C  The difference between the given and expected weight for
           compound is greater 1 mass unit. Check that all hydrogen
           atoms have been taken into account.
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: C47 Eu O10
             Rep.: C47 Eu H35 O10
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
             Calc: C47 Eu O10
             Rep.: C47 Eu H35 O10
PLAT155_ALERT_4_C The Triclinic Unit-Cell is NOT Reduced .........     Please Do !
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Eu1 Check
PLAT741_ALERT_1_C Bond    Calc   1.4069(6), Rep     1.40707 ......    Missing s.u.
             C1       -C2             1_555   1_555 ........     #    1 Check
PLAT741_ALERT_1_C Bond    Calc   1.4013(6), Rep     1.40183 ......    Missing s.u.
             C1       -C6             1_555   1_555 ........     #    2 Check
PLAT741_ALERT_1_C Bond    Calc   1.5029(6), Rep     1.50319 ......    Missing s.u.
             C1       -C7             1_555   1_555 ........     #    3 Check
PLAT741_ALERT_1_C Bond    Calc   1.3996(6), Rep     1.39864 ......    Missing s.u.
             C2       -C3             1_555   1_555 ........     #    4 Check
PLAT741_ALERT_1_C Bond    Calc   1.3974(6), Rep     1.39722 ......    Missing s.u.
             C3       -C4             1_555   1_555 ........     #    5 Check
PLAT741_ALERT_1_C Bond    Calc   1.4001(6), Rep     1.40064 ......    Missing s.u.
             C4       -C5             1_555   1_555 ........     #    6 Check
PLAT741_ALERT_1_C Bond    Calc   1.3996(6), Rep     1.39837 ......    Missing s.u.
             C5       -C6             1_555   1_555 ........     #    7 Check
PLAT741_ALERT_1_C Bond    Calc   1.4199(6), Rep     1.41893 ......    Missing s.u.
             C7       -O1             1_555   1_555 ........     #    8 Check
PLAT741_ALERT_1_C Bond    Calc   1.4141(6), Rep     1.41441 ......    Missing s.u.
             C7       -O2             1_555   1_555 ........     #    9 Check
PLAT741_ALERT_1_C Bond    Calc   2.3160(9), Rep     2.31564 ......    Missing s.u.
```

```
PLAT743_ALERT_1_C Torsion Calc    -0.08(2), Rep       -0.12 ......    Missing s.u.
             C44 -C45 -C46 -C47   1_555  1_555  1_555  1_555      #  159 Check
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
           _chemical_formula_sum and the formula from the _atom_site* data.
           Atom count from _chemical_formula_sum:C47 H35 Eu1 O10
           Atom count from the _atom_site data:  C47 Eu1 O10
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
           From the CIF: _cell_formula_units_Z    1
           From the CIF: _chemical_formula_sum  C47 Eu H35 O10
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         47.00     47.00    0.00
           Eu         1.00      1.00    0.00
           H         35.00      0.00   35.00
           O         10.00     10.00    0.00
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound ..     Please Check
PLAT049_ALERT_1_G Calculated Density Less Than 1.0 gcm-3 .........     0.6589 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C32      ..C44      .       3.12 Ang.
                                                    x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C33      ..C44      .       2.31 Ang.
                                                    x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C33      ..C43      .       3.10 Ang.
                                                    x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C34      ..C44      .       2.57 Ang.
                                                    x,y,-1+z  =      1_554 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C34      ..C43      .       3.00 Ang.
                                                    x,y,-1+z  =      1_554 Check
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found     Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found     Please Check
```

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

 335 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   8 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
   0 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. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

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_PLAT602_I
;
PROBLEM: Solvent Accessible VOID(S) in the Unit-Cell ....          ! Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 26/09/2025; check.def file version of 20/09/2025

---

duplicate check

No duplication found

Datablock I - ellipsoid plot

