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

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Bond precision:   C-C = 0.0004 A          Wavelength=1.54056

Cell:          a=20.911(5)         b=14.804(4)       c=8.847(2)
               alpha=102.352(15)   beta=92.154(16)   gamma=110.660(13)
Temperature:   293 K
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	Calculated	Reported
Volume	2484.1(11)	2484.0(11)
Space group	P 1	P 1
Hall group	P 1	P 1
Moiety formula	C47 Eu O10	C47 Eu O10
Sum formula	C47 Eu O10	C47 Eu O10
Mr	876.44	876.47
Dx,g cm-3	0.586	0.586
Z	1	1
Mu (mm-1)	4.721	4.689
F000	425.0	0.0
F000'	417.51	
h,k,lmax	13,9,5	13,9,5
Nref	2862[1431]	1424
Tmin,Tmax		
Tmin'		

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Correction method= Not given
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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

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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

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
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O7 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..... O9 Check
PLAT741_ALERT_1_C Bond Calc 1.4074(4), Rep 1.40852 ..... Missing s.u.
C1 -C2 1_555 1_555 ..... # 1 Check
PLAT741_ALERT_1_C Bond Calc 1.3975(4), Rep 1.39806 ..... Missing s.u.
C1 -C6 1_555 1_555 ..... # 2 Check
PLAT741_ALERT_1_C Bond Calc 1.4639(4), Rep 1.46365 ..... Missing s.u.
C1 -C7 1_555 1_555 ..... # 3 Check
PLAT741_ALERT_1_C Bond Calc 1.3916(4), Rep 1.39204 ..... Missing s.u.
C2 -C3 1_555 1_555 ..... # 4 Check
PLAT741_ALERT_1_C Bond Calc 1.3975(4), Rep 1.39712 ..... Missing s.u.
C3 -C4 1_555 1_555 ..... # 5 Check
PLAT741_ALERT_1_C Bond Calc 1.4077(4), Rep 1.40817 ..... Missing s.u.
C4 -C5 1_555 1_555 ..... # 6 Check
PLAT741_ALERT_1_C Bond Calc 1.4047(4), Rep 1.40385 ..... Missing s.u.
C5 -C6 1_555 1_555 ..... # 7 Check
PLAT741_ALERT_1_C Bond Calc 1.3536(4), Rep 1.35342 ..... Missing s.u.
C7 -O1 1_555 1_555 ..... # 8 Check
PLAT741_ALERT_1_C Bond Calc 1.2536(3), Rep 1.25338 ..... Missing s.u.
C7 -O2 1_555 1_555 ..... # 9 Check
PLAT741_ALERT_1_C Bond Calc 2.4691(7), Rep 2.46941 ..... Missing s.u.
O1 -EU1 1_555 1_555 ..... # 10 Check
PLAT741_ALERT_1_C Bond Calc 2.5541(7), Rep 2.55397 ..... Missing s.u.
O2 -EU1 1_555 1_555 ..... # 11 Check
PLAT741_ALERT_1_C Bond Calc 1.3998(4), Rep 1.39877 ..... Missing s.u.
C8 -C9 1_555 1_555 ..... # 12 Check
PLAT741_ALERT_1_C Bond Calc 1.4025(4), Rep 1.40325 ..... Missing s.u.
C8 -C13 1_555 1_555 ..... # 13 Check
PLAT741_ALERT_1_C Bond Calc 1.4717(4), Rep 1.47252 ..... Missing s.u.
C8 -C14 1_555 1_555 ..... # 14 Check
PLAT741_ALERT_1_C Bond Calc 1.4045(4), Rep 1.40545 ..... Missing s.u.
C9 -C10 1_555 1_555 ..... # 15 Check
PLAT741_ALERT_1_C Bond Calc 1.3998(4), Rep 1.39891 ..... Missing s.u.

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PLAT743_ALERT_1_C Torsion Calc    -0.29(2), Rep       -0.22 .....    Missing s.u.
             C39 -C40 -C41 -C42   1_555  1_555  1_555  1_555      #  155 Check
PLAT743_ALERT_1_C Torsion Calc     0.49(2), Rep        0.39 .....    Missing s.u.
             C40 -C41 -C42 -C36   1_555  1_555  1_555  1_555      #  156 Check
PLAT743_ALERT_1_C Torsion Calc     0.26(2), Rep        0.17 .....    Missing s.u.
             C37 -C43 -C44 -C45   1_555  1_555  1_555  1_555      #  157 Check
PLAT743_ALERT_1_C Torsion Calc    -0.20(2), Rep       -0.22 .....    Missing s.u.
             C43 -C44 -C45 -C46   1_555  1_555  1_555  1_555      #  158 Check
PLAT743_ALERT_1_C Torsion Calc     0.08(2), Rep        0.19 .....    Missing s.u.
             C44 -C45 -C46 -C47   1_555  1_555  1_555  1_555      #  159 Check
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Alert level G

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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 .........     0.5859 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C17      ..C41      .       2.92 Ang.
                                                  x,1+y,z  =      1_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C17      ..C42      .       3.02 Ang.
                                                  x,1+y,z  =      1_565 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C18      ..C39      .       3.18 Ang.
                                                x,1+y,1+z  =      1_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C39      .       2.00 Ang.
                                                x,1+y,1+z  =      1_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C19      ..C40      .       2.52 Ang.
                                                x,1+y,1+z  =      1_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C20      ..C40      .       2.17 Ang.
                                                x,1+y,1+z  =      1_566 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C20      ..C39      .       2.25 Ang.
                                                x,1+y,1+z  =      1_566 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Eu1       (III)     .       2.77 Info
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
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
 339 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

 339 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  11 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
```

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.

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

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duplicate check

No duplication found

Datablock I - ellipsoid plot

