checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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: 1_a

```
Bond precision:    C-C = 0.0127 A              Wavelength=0.71073

Cell:              a=11.1129(4)        b=11.3025(5)        c=23.0437(8)
                   alpha=76.651(1)     beta=77.617(1)      gamma=71.897(1)
Temperature:       250 K
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	Calculated	Reported
Volume	2644.71(18)	2644.71(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H40 Eu F20 Li O17, C H3	C37 H43 Eu F20 Li O16.19, 0.81(O)
Sum formula	C37 H43 Eu F20 Li O17	C37 H43 Eu F20 Li O17
Mr	1298.63	1298.61
Dx,g cm-3	1.631	1.631
Z	2	2
Mu (mm-1)	1.319	1.319
F000	1294.0	1294.0
F000'	1294.83	
h,k,lmax	17,17,35	17,17,35
Nref	20563	18047
Tmin,Tmax	0.876,0.974	0.592,0.747
Tmin'	0.876	

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Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.747
AbsCorr = MULTI SCAN


Data completeness= 0.878              Theta(max)= 33.381


R(reflections)= 0.0744( 11945)                        wR2(reflections)=
                                                      0.2389( 18047)

S = 1.030                      Npar= 727
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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

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PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ      Please Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....        2.09 Report
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F1        --C4      .        5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F3        --C5      .        6.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F5        --C5      .        6.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F9        --C14     .        6.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F10       --C14     .        5.2 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F16       --C31     .        6.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     F18       --C32     .        6.9 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     O17       --C37     .        5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for     C31       --C32     .        6.7 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F20        --C32     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4         --C8      .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O11        --C25     .       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O15A       --C33     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C4         --C5      .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13        --C14     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33        --C36     .       0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O14 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        C20 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Eu1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O12 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O16 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O17 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C31 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        C9       0.103 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.01274 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C13      - C14      .       1.43 Ang.
PLAT360_ALERT_2_C Short  C(sp3)-C(sp3) Bond  C31      - C32      .       1.38 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C33      - C36      .       1.67 Ang.
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4    Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.433 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         67 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.45Ang From F19            2.30 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.18Ang From F10            1.73 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.78Ang From C24            1.68 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.54Ang From F4             1.59 eA-3
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⬤ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite        4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       31 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large     0.14 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)     0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
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PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        9 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0200 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for     O15      --C33     .      7.8 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for     O11A     --C24     .      6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for     O11A     --C27     .      7.9 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of    C5 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C14 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C23 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of   C32 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )     4% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O4A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....  O11A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....  O15A Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for   C32 Check
PLAT344_ALERT_2_G Unusual sp?      Angle Range in Solvent/Ion for     C9 Check
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O4      .   107.7 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O15     .   109.4 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3      ..C9      .     2.55 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C2      ..C9      .     3.18 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C3      ..C9      .     2.60 Ang.
                                              x,y,z  =     1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C7      ..C9      .     3.10 Ang.
                                              x,y,z  =     1_555 Check
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C6      --C9        1.77 Ang.
PLAT793_ALERT_4_G Model has Chirality at C15       (Centro SPGR)     R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Eu1     (III)     .   3.49 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............  185 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).    2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600  2446 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File    1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........  1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.    0 Info
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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
  41 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  37 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  53 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
  13 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* 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.

PLATON version of 28/11/2022; check.def file version of 28/11/2022

NOMOVE_FORCED

Prob = 50
Temp = 250

45 Y

PLATON-Dec 16 15:35:06 2022 - (281122)

Z 28   1_a   P -1   R = 0.07   RES= 0 -29 X