checkCIF/PLATON report

Structure factors have been supplied for datablock(s) lsn010

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: lsn010

```
Bond precision:  C-C = 0.0132 A          Wavelength=0.71073

Cell:          a=11.8993(6)       b=12.9623(6)     c=16.1082(8)
               alpha=110.744(5)   beta=94.010(4)   gamma=114.162(5)
Temperature:   100 K
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	Calculated	Reported
Volume	2051.6(2)	2051.6(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H5 Er F33 O8 P	C33 H5 Er F33 O8 P
Sum formula	C33 H5 Er F33 O8 P	C33 H5 Er F33 O8 P
Mr	1354.60	1354.60
Dx,g cm-3	2.193	2.193
Z	2	2
Mu (mm-1)	2.286	2.286
F000	1294.0	1294.0
F000’	1295.07	
h,k,lmax	14,15,19	14,15,19
Nref	7523	7318
Tmin,Tmax	0.760,0.892	0.490,1.000
Tmin’	0.504	

```
Correction method= # Reported T Limits: Tmin=0.490 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.973          Theta(max)= 25.348

R(reflections)= 0.0593( 6368)     wR2(reflections)= 0.1129( 7318)

S = 1.207                 Npar= 686
```

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

```
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......      0.973 Note
PLAT213_ALERT_2_C Atom F2              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom F8              has ADP max/min Ratio .....        3.3 prolat
PLAT220_ALERT_2_C Large Non-Solvent  F     Ueq(max)/Ueq(min) Range       3.5 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C9 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01317 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      5.947 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.600        198 Report
PLAT971_ALERT_2_C Check Calcd Residual Density  1.00A From     Er1       1.58 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  1.02A From      O8       0.71 eA-3
PLAT975_ALERT_2_C Check Calcd Residual Density  0.92A From      O7       0.69 eA-3
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Alert level G

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PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...         76 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          2 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      13.25 Why ?
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C4 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C14 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F5     ..  C25     ..       2.95 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F7     ..  F23     ..       2.69 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F16    ..  F22     ..       2.81 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F20    ..  F28     ..       2.79 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F25    ..  F33     ..       2.64 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F29    ..  F30     ..       2.84 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        699 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Th(Min) ...          2 Report
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600          6 Note
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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
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
   6 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. 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 19/11/2015; check.def file version of 17/11/2015

Datablock lsn010 - ellipsoid plot