checkCIF/PLATON report

Structure factors have been supplied for datablock(s) kds367_pl

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: kds367_pl

```
Bond precision:   C-C = 0.0032 A          Wavelength=0.71073

Cell:             a=14.9027(3)     b=15.6143(3)         c=16.1279(4)
                  alpha=90         beta=108.471(1)      gamma=90
Temperature:      150 K
```

	Calculated	Reported
Volume	3559.55(13)	3559.55(13)
Space group	I 2/c	I 1 2/c 1
Hall group	-I 2yc	-I 2yc
Moiety formula	C10 H12 Eu N9 O10	C10 H12 Eu N9 O10
Sum formula	C10 H12 Eu N9 O10	C10 H12 Eu N9 O10
Mr	570.26	570.25
Dx,g cm-3	2.128	2.128
Z	8	8
Mu (mm-1)	3.601	3.601
F000	2224.0	2224.0
F000'	2223.78	
h,k,lmax	21,22,23	21,22,22
Nref	5440	5332
Tmin,Tmax	0.506,0.750	0.583,0.746
Tmin'	0.482	

```
Correction method= # Reported T Limits: Tmin=0.583 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.980           Theta(max)= 30.529

R(reflections)= 0.0184( 4589)                    wR2(reflections)=
                                                 0.0414( 5332)
S = 1.091                  Npar= 277
```

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 B

```
PLAT430_ALERT_2_B Short Inter D...A Contact  O3       ..O6       .       2.83 Ang.
                                          -1/2+x,-1/2-y,z  =      8_445 Check
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Author Response: The oxygen atoms belong to nitrates; this is a feature of the crystal packing.

Alert level C

```
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1       --N7       .        5.4 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O5       --N8       .        6.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O7       --N9       .        7.0 s.u.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
              C10 H12 Eu N9 O10
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          7 Report
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
```

Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          3 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.36 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O1       .       10.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O2       .       20.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O4       .        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O5       .       11.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Eu1      --O7       .       12.6 s.u.
PLAT432_ALERT_2_G Short Inter X...Y Contact  O6       ..N7       .       2.76 Ang.
                                          1/2+x,-1/2-y,z  =      8_545 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         99 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          9 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          4 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   6 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

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

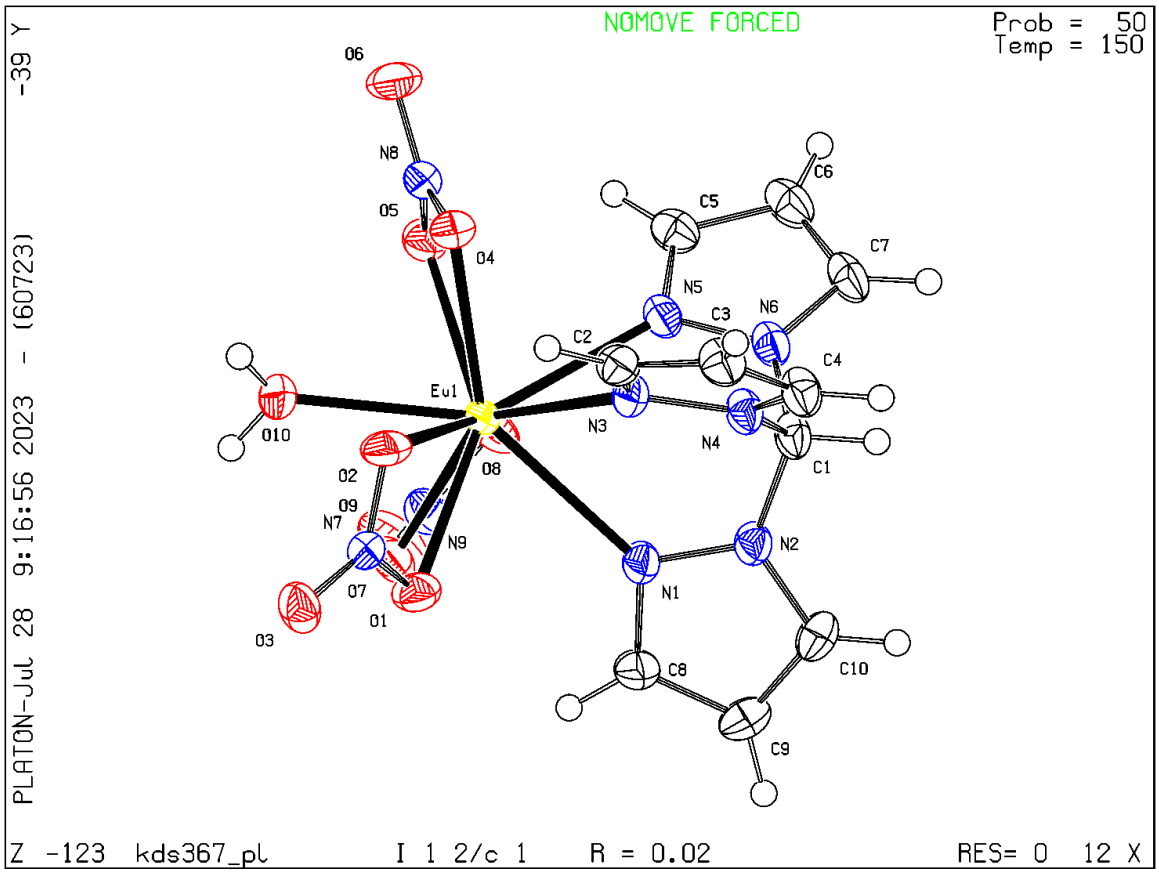
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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 06/07/2023; check.def file version of 30/06/2023

Datablock kds367_pl - ellipsoid plot