checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ppr2

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: ppr2

Bond precision: C-C = 0.0174 A Wavelength=0.71073

Cell: a=21.596(3) b=17.912(2) c=18.668(2)
alpha=90 beta=115.419(4) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	6522.2(14)	6522.3(14)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H24 Eu2 F18 N12 O20 S6, 0.682(C4 H10 O), 2(C2 H3 N)	2(C13 H12 Eu F9 N6 O10 S3), 0.682(C4 H10 O), 2(C2 H3 N)
Sum formula	C32.73 H36.82 Eu2 F18 N14 O20.68 S6	C32.90 H37.24 Eu2 F18 N14 O20.73 S6
Mr	1795.53	1798.66
Dx,g cm-3	1.829	1.832
Z	4	4
Mu (mm-1)	2.224	2.224
F000	3522.6	3530.0
F000'	3526.62	
h,k,lmax	26,21,22	26,21,22
Nref	12484	12125
Tmin,Tmax	0.766,0.935	0.602,0.745
Tmin'	0.766	

Correction method= # Reported T Limits: Tmin=0.602 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.971 Theta(max)= 25.742

R(reflections)= 0.0612(8725)

wR2(reflections)= 0.1542(12125)

S = 1.050 Npar= 841

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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PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       3.13 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent .........          5 Check
             O1S     C5S     C6S     C7S     C8S
PLAT213_ALERT_2_C Atom F4              has ADP max/min Ratio .....        3.9 prolat
PLAT213_ALERT_2_C Atom F6              has ADP max/min Ratio .....        3.1 prolat
PLAT213_ALERT_2_C Atom C13             has ADP max/min Ratio .....        3.1 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference F4       --C12      .       0.17 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         S5 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        C1S Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01743 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd.  #          1 Note
             C26 H24 Eu2 F18 N12 O20 S6
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        222 Report
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Alert level G

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FORMU01_ALERT_1_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and _chemical_formula_moiety. This is
            usually due to the moiety formula being in the wrong format.
            Atom count from _chemical_formula_sum:   C32.9 H37.24 Eu2 F18 N14 O20.
            Atom count from _chemical_formula_moiety:C32.72800 H36.82 Eu2 F18 N14
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:C32.9 H37.24 Eu2 F18 N14 O20.73
            Atom count from the _atom_site data:  C32.72799 H36.81999 Eu2 F18 N14
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  C32.90 H37.24 Eu2 F18 N14 O20.73 S
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           C         131.60    130.91    0.69
           H         148.96    147.28    1.68
           Eu          8.00      8.00    0.00
           F          72.00     72.00    0.00
           N          56.00     56.00    0.00
           O          82.92     82.73    0.19
           S          24.00     24.00    0.00
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...          3 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          4 Report
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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      92.14 Why ?
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C2 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C12 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C18 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of         C3 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C10 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C24 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )        100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... (Resd  3  )      10.23 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....            16 Note
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             C5S     -C6S     -H6SB       1_555  1_555  1_555     #  239 Check
PLAT722_ALERT_1_G Angle   Calc      108.00, Rep      109.50 Dev...       1.50 Degree
             C5S     -C6S     -H6SC       1_555  1_555  1_555     #  240 Check
PLAT722_ALERT_1_G Angle   Calc      111.00, Rep      109.50 Dev...       1.50 Degree
             H6SA    -C6S     -H6SC       1_555  1_555  1_555     #  242 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #           3 Note
             C4 H10 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #           4 Note
             C2 H3 N
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          18 Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..           ! Info
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          58 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....           1 Note
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law         [ 2 0 1] Est.d BASF       0.11 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          10 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........         1.0 Low
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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
 14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 30 **ALERT level G** = General information/check it is not something unexpected

 10 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
  7 ALERT type 3 Indicator that the structure quality may be low
 11 ALERT type 4 Improvement, methodology, query or suggestion
  2 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 ppr2 - ellipsoid plot