

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: 170623e

Bond precision: C-C = 0.0157 Å Wavelength=0.71073

Cell: a=14.3022(13) b=34.152(3) c=19.4743(17)
 alpha=90 beta=106.772(2) gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	9107.6(14)	9107.6(14)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	?
Moiety formula	2(C76 H56 Eu Fe4 N8 O20), 7(C5 H5 N), 2(C5 H6 N)	?
Sum formula	C197 H159 Eu2 Fe8 N25 O40	C98.50 H79.50 Eu Fe4 N12.50 O20
Mr	4267.24	2133.61
Dx, g cm ⁻³	1.556	1.556
Z	2	4
Mu (mm ⁻¹)	1.381	1.381
F000	4340.0	4340.0
F000'	4346.55	
h,k,lmax	17,40,23	17,40,23
Nref	16068	16024
Tmin,Tmax	0.594,0.679	0.608,0.863
Tmin'	0.570	

Correction method= # Reported T Limits: Tmin=0.608 Tmax=0.863
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.020

R(reflections)= 0.0594(10074) wR2(reflections)= 0.1646(16024)

S = 1.020 Npar= 1225

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

CRYSC01_ALERT_1_C	No recognised colour has been given for crystal colour.	
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.2 Ratio
PLAT234_ALERT_4_C	Large Hirshfeld Difference N7 --C67	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference N8 --C76	0.16 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C69 --C70	0.19 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C70 --C71	0.19 Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C70	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of C75	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of N7	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of C92	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of C90	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C93	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C95	Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of C91	Check
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.6 Note
PLAT331_ALERT_2_C	Small Average Phenyl C-C Dist C37 -C42	1.37 Ang.
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01569 Ang.
PLAT369_ALERT_2_C	Long C(sp2)-C(sp2) Bond C88 - C89 .	1.53 Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H92 ..H97	2.03 Ang.
PLAT411_ALERT_2_C	Short Inter H...H Contact H96 ..H99	2.11 Ang.

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	41 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	137 Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N13 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C98 Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H98 Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	27% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact N12 ..C99	2.47 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact N12 ..C97	2.55 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C92 ..C97	3.06 Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C96 ..C99	3.12 Ang.
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # C5 H5 N	3 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Eu1 (III) .	3.28 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.02 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe2 (III) .	3.09 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe3 (III) .	3.08 Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe4 (III) .	3.03 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	4020 Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

0 **ALERT level B** = A potentially serious problem, consider carefully

20 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

21 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

15 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
15 ALERT type 4 Improvement, methodology, query or suggestion
7 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 23/04/2018; check.def file version of 23/04/2018

