

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_IALVB88_0m_aa

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: mo_IALVB88_0m_aa

Bond precision:	C-C = 0.0086 Å	Wavelength=0.71073
Cell:	a=11.1009(6)	b=21.8025(12) c=18.7796(11)
	alpha=90	beta=106.930(3) gamma=90
Temperature:	100 K	
	Calculated	Reported
Volume	4348.2(4)	4348.2(4)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C40 H24 Eu F12 O8, C5 H6 N	C40 H24 Eu F12 O8, C5 H6 N
Sum formula	C45 H30 Eu F12 N O8	C45 H30 Eu F12 N O8
Mr	1092.67	1092.66
Dx, g cm ⁻³	1.669	1.669
Z	4	4
Mu (mm ⁻¹)	1.549	1.549
F000	2168.0	2168.0
F000'	2168.87	
h, k, lmax	13, 25, 22	12, 25, 22
Nref	7641	6112
Tmin, Tmax	0.863, 0.943	0.473, 0.746
Tmin'	0.633	

Correction method= # Reported T Limits: Tmin=0.473 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.800 Theta(max)= 24.999

R(reflections)= 0.0324(3719)	wR2(reflections)=
S = 0.832	0.0505(6112)
Npar= 568	

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 A**

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.800 Why?

Author Response: The crystals were found to be weakly diffracting and as a result, reflections did not extend out as far in theta as what would normally be considered desirable for small molecules.

 **Alert level B**

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.595 1496 Report

Author Response: Due to the quality of the some reflections below theta min were affected by the beamstop, they haven't been taken into account but this doesn't affect the refinement

 **Alert level C**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137

Author Response: The elevated values of _diffn_reflms_av_R_equivalents is due to the poor crystal diffraction because the crystal was very thin. Other attempts of crystallization were done, but no single crystals of better quality were obtained.

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.9 Ratio

Author Response: Due to the quality of the crystal there was little dynamic disorder

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.3 Note

Author Response: Due to the quality of the crystal there was little dynamic disorder

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.00857 Ang.

Author Response: The isolated crystals were very thin and diffracted weakly at high angles, for this reason the C-C Bonds are low precision

PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).

6 Note

Author Response: Due to the poor crystal diffraction because the crystal was very thin.

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.60A From N1

-0.40 eA-3

Author Response: Due to the quality of the crystal



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2	Note
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1	Report
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12	0.137	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1	Report
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C11	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C21	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C31	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Eu1 (III) .	3.48	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	1	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	38%	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	1.0	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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- 1 **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

- 1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
9 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

