

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mes11_0m

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: mes11_0m

Bond precision: C-C = 0.0077 Å

Wavelength=0.71073

Cell: a=11.042 (4) b=15.985 (5) c=16.261 (5)
 alpha=106.206 (17) beta=95.895 (18) gamma=96.034 (18)
Temperature: 299 K

	Calculated	Reported
Volume	2714.5 (16)	2714.5 (16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C30 H22 Eu N8 O6, C15 H11 Eu N7 O12, 2(C2 H3 N)	C30 H22 Eu N8 O6, C15 H11 Eu N7 O12, 2(C2 H3 N)
Sum formula	C49 H39 Eu2 N17 O18	C49 H39 Eu2 N17 O18
Mr	1457.91	1457.91
Dx, g cm ⁻³	1.784	1.784
Z	2	2
Mu (mm ⁻¹)	2.380	2.380
F000	1444.0	1444.0
F000'	1443.97	
h, k, lmax	14, 21, 21	14, 21, 21
Nref	13788	13317
Tmin, Tmax	0.720, 0.877	0.647, 0.746
Tmin'	0.706	

Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.966

Theta(max)= 28.510

R(reflections)= 0.0415 (10079)

wR2(reflections)=
0.1003 (13317)

S = 1.021

Npar= 777

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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N14 Check

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C13 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of 014 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Eu02 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C48 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including N15 0.103 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 192 Report
3 0 0, 5 0 0, 1 1 0, 2 1 0, 4 1 0, 5 2 0,
-2 3 0, -1 3 0, 0 4 0, 1 4 0, 3 4 0, -3 5 0,
0 5 0, 2 5 0, -2 6 0, -1 7 0, 0 7 0, 1 8 0,
-1 15 0, -2 -7 1, 3 -7 1, -1 -6 1, 0 -6 1, -2 -5 1,
-3 -4 1, -1 -4 1, 1 -4 1, 2 -4 1, -4 -3 1, 4 -3 1,
0 -2 1, 1 -2 1, -4 -1 1, -3 -1 1, 1 -1 1, -3 0 1,
-2 0 1, 1 0 1, 3 0 1, -1 1 1, 0 1 1, 4 1 1,
0 2 1, 1 2 1, 3 2 1, -2 3 1, -2 4 1, -4 6 1,
1 6 1, -3 7 1, -2 14 1, 1 -7 2, 2 -6 2, -4 -5 2,
4 -5 2, -3 -4 2, -1 -3 2, -5 -2 2, -2 -2 2, -1 -2 2,
1 -2 2, 5 -2 2, -1 -1 2, 4 -1 2, -4 0 2, 0 0 2,
1 0 2, 5 0 2, 0 1 2, 1 1 2, 4 1 2, 3 2 2,
2 3 2, -3 5 2, 0 7 2, -1 14 2, 1-16 3, 2 -8 3,
-1 -7 3, -4 -5 3, 1 -5 3, 9 -5 3, -5 -4 3, -4 -3 3,
-4 -2 3, 0 -2 3, 1 -2 3, -3 -1 3, 1 -1 3, 2 -1 3,
-5 0 3, -2 0 3, 3 0 3, -1 1 3, 2 1 3, 4 1 3,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 77 Note
5 0 0, 1 1 0, 5 2 0, -2 3 0, -1 3 0, 0 4 0,
1 4 0, -3 5 0, 0 5 0, 2 5 0, -2 6 0, -1 7 0,
1 8 0, -2 -7 1, 3 -7 1, -1 -6 1, 2 -4 1, -4 -3 1,
0 -2 1, -3 -1 1, 1 -1 1, -3 0 1, -2 0 1, 3 0 1,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
11-15 7,

Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Eu01 --O4 . 6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Eu02 --O7 . 10.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Eu02 --O12 . 6.0 s.u.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3 Note
Eu01 Eu02 N011
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
1 0 0, 0 1 0, 0 -1 1, 0 0 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 275 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 9 Note
2 -4 5, 2 -1 3, 4 -1 2, 0 -2 3, 2 1 0, 3 -4 5,

2 -5 5, 1 -2 3, 3-18 12,
 PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 2.3 Low
 PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.425 Note
 Predicted wR2: Based on SigI**2 7.04 or SHELX Weight 9.82
 PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 3 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 10 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 12 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
 4 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* 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.

