

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1_a

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: 1_a

Bond precision: C-C = 0.0061 Å Wavelength=0.71073

Cell: a=10.4566(4) b=13.7470(5) c=22.4166(8)
 alpha=98.286(1) beta=100.441(1) gamma=90.463(1)
Temperature: 100 K

	Calculated	Reported
Volume	3133.9(2)	3133.9(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H44 Eu F36 Li O17	C45 H44 Eu F36 Li O16.64, 0.36(O)
Sum formula	C45 H44 Eu F36 Li O17	C45 H44 Eu F36 Li O17
Mr	1699.71	1699.70
Dx, g cm ⁻³	1.801	1.801
Z	2	2
Mu (mm ⁻¹)	1.171	1.171
F000	1680.0	1680.0
F000'	1681.39	
h, k, lmax	16, 21, 34	15, 21, 34
Nref	24256	21295
Tmin, Tmax	0.869, 0.889	0.596, 0.747
Tmin'	0.704	

Correction method= # Reported T Limits: Tmin=0.596 Tmax=0.747
AbsCorr = MULTI SCAN

Data completeness= 0.878 Theta(max)= 33.324

R(reflections)= 0.0534(17976)

wR2(reflections)=
0.1429(21295)

S = 1.049

Npar= 942

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.24Ang From F11 3.19 eA-3

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ... 2.02 Report
PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 F Ueq(max)/Ueq(min) Range 5.3 Ratio
PLAT220_ALERT_2_C NonSolvent Resd 1 O Ueq(max)/Ueq(min) Range 4.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C19 --C22 . 5.7 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F8 --C7 . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8A --C22 . 0.19 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT767_ALERT_4_C INS Embedded LIST 6 Instruction Should be LIST 4 Please Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min). 5 Note
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 81 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99Ang From F16 2.06 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.50Ang From F11 1.93 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.43Ang From F14 1.90 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.19Ang From F14 1.82 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.02Ang From F11 1.70 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17 . -0.34 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 8 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 7.79 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records 2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 2 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0200 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par 0.0030 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar 0.0060 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for O8 --C19 . 8.0 s.u.
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C7 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 C29 Check
PLAT242_ALERT_2_G Low 'MainMol' Ueq as Compared to Neighbors of C40 Check
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 3% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 04A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 08A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) 015A Check
PLAT431_ALERT_2_G Short Inter HL..A Contact F17 ..O8A . 2.66 Ang.
1-x,-y,1-z = 2_656 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F16 ..F18 . 2.62 Ang.
-x,-y,1-z = 2_556 Check

PLAT434_ALERT_2_G	Short Inter HL..HL Contact F18	..F18	.	2.65	Ang.
		-x,-y,1-z =		2_556	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact F18	..F23	.	2.81	Ang.
		-1+x,-1+y,z =		1_445	Check
PLAT793_ALERT_4_G	Model has Chirality at C8	(Centro SPGR)		R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C19	(Centro SPGR)		S	Verify
PLAT794_ALERT_5_G	Tentative Bond Valency for Eu1	(III)	.	3.47	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints		41	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary				Please Do !
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600		2829	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File			7	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity		1.8	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			0	Info

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 31 ALERT type 2 Indicator that the structure model may be wrong or deficient
 8 ALERT type 3 Indicator that the structure quality may be low
 10 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.

