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 = 0.0049 A Wavelength=0.71073

Cell: a=10.4696(13) b=13.756(2) c=22.417(3)
alpha=98.181(5) beta=100.306(5) gamma=90.527(6)
Temperature: 100 K

	Calculated	Reported
Volume	3142.1(7)	3142.1(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H44 F36 Gd Li O17	C45 H44 F36 Gd Li O16.68, 0.32(O)
Sum formula	C45 H44 F36 Gd Li O17	C45 H44 F36 Gd Li O17
Mr	1704.99	1704.99
Dx,g cm-3	1.802	1.802
Z	2	2
Mu (mm-1)	1.226	1.226
F000	1682.0	1682.0
F000'	1683.37	
h,k,lmax	16,21,34	15,20,34
Nref	23998	21278
Tmin,Tmax	0.863,0.907	0.592,0.747
Tmin'	0.736	

Correction method= # Reported T Limits: Tmin=0.592 Tmax=0.747
AbsCorr = MULTI SCAN

Data completeness= 0.887 Theta(max)= 33.164

R(reflections)= 0.0453(18791) wR2(reflections)= 0.1184(21278)

S = 1.050 Npar= 956

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

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PLAT971_ALERT_2_B Check Calcd Resid. Dens.  1.26Ang From F28            2.66 eA-3
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Alert level C

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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       4.0 Ratio
PLAT220_ALERT_2_C NonSolvent   Resd 1  F   Ueq(max)/Ueq(min) Range       4.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F5       --C6       .       6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C8       --C11      .       7.0 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C41      --C44      .       7.0 s.u.
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
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        74 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From F35            2.15 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.57Ang From F30            1.90 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.15Ang From C37            1.55 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17       .     -0.34 eA-3
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       13 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       12 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      6.61 Why ?
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
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records        3 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        3 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        5 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par   0.0080 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar   0.0160 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par   0.0050 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for First Par   0.0080 Report
PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar   0.0160 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F9B      --C7       .       5.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O16      --C41      .      10.5 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  )        4% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O4A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....      O16A Check
PLAT431_ALERT_2_G Short Inter HL..A Contact  F36      ..O16A     .      2.66 Ang.
                                              1-x,-y,1-z  =     2_656 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F11      ..F32      .      2.83 Ang.
                                                x,1+y,z  =     1_565 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F15      ..F34      .      2.83 Ang.
                                              1+x,1+y,z  =     1_665 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F34      ..F35      .      2.71 Ang.
                                              -x,-y,1-z  =     2_556 Check
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PLAT434_ALERT_2_G Short Inter HL..HL Contact F34      ..F34      .       2.71 Ang.
                                                  -x,-y,1-z  =      2_556 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          4 Note
PLAT793_ALERT_4_G Model has Chirality at C8          (Centro SPGR)     R Verify
PLAT793_ALERT_4_G Model has Chirality at C41         (Centro SPGR)     S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1       (III)     .     3.46 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....           112 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .  Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).      3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600   2583 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File      4 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
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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
38 **ALERT level G** = General information/check it is not something unexpected

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

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock 1_a - ellipsoid plot