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

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Bond precision:    C-C = 0.0133 A            Wavelength=0.71073

Cell:             a=11.1199(7)        b=11.3337(7)        c=23.0251(13)
                  alpha=76.524(2)    beta=77.560(2)     gamma=71.624(2)
Temperature:      250 K

                  Calculated                Reported
Volume            2646.2(3)                 2646.2(3)
Space group       P -1                      P -1
Hall group        -P 1                      -P 1
Moiety formula    C37 H44 F20 Gd Li O17     C37 H44 F20 Gd Li O16.44,
                                            0.56(O)
Sum formula       C37 H44 F20 Gd Li O17     C37 H44 F20 Gd Li O17
Mr                1304.91                   1304.91
Dx,g cm-3         1.638                     1.638
Z                 2                         2
Mu (mm-1)         1.386                     1.386
F000              1298.0                    1298.0
F000'             1298.81
h,k,lmax          15,16,32                  15,16,32
Nref              16142                     16007
Tmin,Tmax         0.745,0.973               0.584,0.747
Tmin'             0.730

Correction method= # Reported T Limits: Tmin=0.584 Tmax=0.747
AbsCorr = MULTI SCAN

Data completeness= 0.992            Theta(max)= 30.507


R(reflections)= 0.0759( 11609)                      wR2(reflections)=
                                                    0.2349( 16007)
S = 1.034                     Npar= 759
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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**
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PLAT220_ALERT_2_C NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range       3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F22A    --C22     .       5.8 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F23A    --C23     .       6.3 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    F23C    --C23     .       5.6 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C15     --C18     .       5.1 s.u.
PLAT230_ALERT_2_C Hirshfeld Test Diff for    C24     --C27     .       5.6 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14A    --C14     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F14C    --C14     .       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F22B    --C22     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F23B    --C23     .       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F32A    --C32     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F32B    --C32     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4      --C8      .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8      --C15     .       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O8      --C17     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O12     --C24     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13     --C14     .       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C22     --C23     .       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31     --C32     .       0.20 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C2 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   Gd1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C4 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C13 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C22 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of   C31 Check
PLAT309_ALERT_2_C Single Bonded Oxygen (C-O > 1.3 Ang) ..........   O4A Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............  0.01332 Ang.
PLAT361_ALERT_2_C Long   C(sp3)-C(sp3) Bond  C15     - C18     .      1.74 Ang.
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       64 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .       1 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.95Ang From F23B       2.31 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.26Ang From F23B       2.05 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.87Ang From F14A       1.58 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.22Ang From F32C       1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.58Ang From F23A      -1.61 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Gd1    1.26 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H17B      .   -0.32 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       28 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       23 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large   0.13 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)   0.002 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records        4 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        6 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records        1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records        7 Report
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PLAT192_ALERT_3_G A Non-default DELU Restraint Value for SecondPar    0.0200 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C6        --C9      .      5.2 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C8        --C6A     .      6.6 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of      C5 Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of     C14 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )      8% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O8A Check
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) .....   O12A Check
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond C21      - C24     .     1.55 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond C24      - C27     .     1.69 Ang.
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O4      .    108.7 Degree
PLAT398_ALERT_2_G Deviating  C-O-C   Angle From 120 for O8      .    108.5 Degree
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H7A      ..H9C      .     2.04 Ang.
                                                  x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H8C      ..H7AC     .     1.92 Ang.
                                                  x,y,z  =      1_555 Check
PLAT413_ALERT_2_G Short Inter XH3 .. XHn      H2       ..H7AB     .     2.09 Ang.
                                               -x,-y,1-z  =      2_556 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........    3 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C15       --C18     1.74 Ang.
PLAT793_ALERT_4_G Model has Chirality at C15        (Centro SPGR)     R Verify
PLAT793_ALERT_4_G Model has Chirality at C33        (Centro SPGR)     R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Gd1       (III)     .   3.50 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............   201 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).     2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600    70 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....     3 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File     1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........   2.1 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
   0 ALERT level B = A potentially serious problem, consider carefully
  38 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  37 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  40 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
  23 ALERT type 4 Improvement, methodology, query or suggestion
   1 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.

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

Datablock 1_a - ellipsoid plot