checkCIF/PLATON report

Structure factors have been supplied for datablock(s) z11

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: z11

```
Bond precision:  C-C = 0.0137 A          Wavelength=1.54178

Cell:         a=11.0001(4)        b=14.8467(5)     c=22.0163(7)
              alpha=102.4725(16)  beta=98.0625(16) gamma=106.5187(17)
Temperature: 240 K
```

	Calculated	Reported
Volume	3286.8(2)	3286.8(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H44 Dy F36 Li O17	?
Sum formula	C45 H44 Dy F36 Li O17	C45 H44 Dy F36 Li O17
Mr	1710.24	1710.24
Dx,g cm-3	1.728	1.728
Z	2	2
Mu (mm-1)	7.599	7.599
F000	1686.0	1686.0
F000’	1674.91	
h,k,lmax	13,17,26	13,17,26
Nref	11941	11760
Tmin,Tmax	0.271,0.320	
Tmin’	0.205	

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Correction method= Not given

Data completeness= 0.985          Theta(max)= 67.873

R(reflections)= 0.0821( 10270)    wR2(reflections)= 0.2144( 11760)

S = 1.055                 Npar= 901
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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 B

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PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C12D Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C15B Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C18C Check
PLAT242_ALERT_2_B Low    'MainMol' Ueq as Compared to Neighbors of       C18D Check
```

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.138
PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12 .........      0.138 Report
PLAT057_ALERT_3_C Correction for Absorption Required   RT(exp) ...       1.18 Do !
PLAT213_ALERT_2_C Atom F14D           has ADP max/min Ratio .....        3.7 prolat
PLAT213_ALERT_2_C Atom F19D           has ADP max/min Ratio .....        4.0 prolat
PLAT213_ALERT_2_C Atom F20D           has ADP max/min Ratio .....        3.9 prolat
PLAT220_ALERT_2_C Non-Solvent  Resd 1  C   Ueq(max)/Ueq(min) Range       4.0 Ratio
PLAT220_ALERT_2_C Non-Solvent  Resd 1  F   Ueq(max)/Ueq(min) Range       4.8 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O7A      --C8A      .       6.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F17D     --C15D     .      0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F20B     --C18B     .      0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O7C      --C8C      .      0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C3A      --C4A      .      0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of        O7A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O1S Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O5A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        O7B Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C12A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C12B Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C12C Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C15A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C15C Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C15D Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C18A Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of       C18B Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including        Dy      0.139 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............    0.01366 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .        47 Ang**3
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       140 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00A   From Dy            1.72 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.58A   From F24B          1.70 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.11A   From Dy            1.55 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.01A   From Dy            1.54 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.99A   From O5D           0.71 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H1SC           -0.43 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.         0 Info
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         20 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        100 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large      0.17 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          9 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records          1 Report
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C21A Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C21B Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C21C Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of       C21D Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C18B Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O7A          102.4 Degree
PLAT434_ALERT_2_G Short Inter HL..HL Contact F20D     ..F24B           2.75 Ang.
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                                                x,-1+y,z  =      1_545 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          43 Note
PLAT793_ALERT_4_G Model has Chirality at C3A         (Centro SPGR)      S Verify
PLAT793_ALERT_4_G Model has Chirality at C3D         (Centro SPGR)      S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Dy        (III)     .    3.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .....            355 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     74% Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600     40 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...      2 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   4 ALERT level B = A potentially serious problem, consider carefully
  36 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  22 ALERT level G = General information/check it is not something unexpected

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

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock z11 - ellipsoid plot