checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 252

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: 252

Bond precision: C-C = 0.0087 A Wavelength=1.54178

Cell: a=11.1190(3) b=11.3357(3) c=22.9094(6)
alpha=76.297(1) beta=77.360(1) gamma=71.388(1)
Temperature: 296 K

	Calculated	Reported
Volume	2626.27(12)	2626.27(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H41 Dy F19.50 Li O17, 0.5(F), C H3	?
Sum formula	C37 H44 Dy F20 Li O17	C37 H44 Dy F20 Li O17
Mr	1310.16	1310.16
Dx,g cm-3	1.657	1.657
Z	2	2
Mu (mm-1)	8.848	8.848
F000	1302.0	1302.0
F000’	1288.35	
h,k,lmax	13,13,27	13,13,27
Nref	9540	9407
Tmin,Tmax	0.687,0.767	
Tmin’	0.253	

Correction method= Not given

Data completeness= 0.986 Theta(max)= 67.761

R(reflections)= 0.0402(8914) wR2(reflections)= 0.1103(9407)

S = 1.037 Npar= 805

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

PLAT215_ALERT_3_B Disordered F9A has ADP max/min Ratio ..... 4.2 Note
PLAT215_ALERT_3_B Disordered F9C has ADP max/min Ratio ..... 4.3 Note
PLAT230_ALERT_2_B Hirshfeld Test Diff for O14D --C15D . 30.9 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for O16C --C17C . 20.0 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C13B --C18B . 13.6 s.u.
PLAT230_ALERT_2_B Hirshfeld Test Diff for C13C --C18C . 8.0 s.u.
PLAT234_ALERT_4_B Large Hirshfeld Difference F7D --C6D . 0.30 Ang.
PLAT234_ALERT_4_B Large Hirshfeld Difference F8C --C6C . 0.28 Ang.
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of O14D Check
PLAT260_ALERT_2_B Large Average Ueq of Residue Including F8DA 0.303 Check

Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.12 Do !
PLAT213_ALERT_2_C Atom O16B has ADP max/min Ratio ..... 3.8 prolat
PLAT213_ALERT_2_C Atom C15B has ADP max/min Ratio ..... 3.4 prolat
PLAT215_ALERT_3_C Disordered F1# has ADP max/min Ratio ..... 3.4 Note
PLAT215_ALERT_3_C Disordered F3# has ADP max/min Ratio ..... 3.1 Note
PLAT215_ALERT_3_C Disordered F4D has ADP max/min Ratio ..... 3.4 Note
PLAT215_ALERT_3_C Disordered F5D has ADP max/min Ratio ..... 3.6 Note
PLAT215_ALERT_3_C Disordered F8A has ADP max/min Ratio ..... 3.4 Note
PLAT215_ALERT_3_C Disordered F9D has ADP max/min Ratio ..... 3.7 Note
PLAT215_ALERT_3_C Disordered F13# has ADP max/min Ratio ..... 4.0 Note
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 F Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.6 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for O16B --C13B . 5.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference F7DA --C6D . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F5C --C3C . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F8B --C6B . 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F8D --C6D . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F9B --C6B . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F7AA --C6A . 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F8AA --C6A . 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13D --C18D . 0.17 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C6C Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C10B 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 O14B Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of O14C Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3A Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C3B 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 C13B Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Dy 0.118 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including C17B 0.135 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00871 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C3C - C6C . 1.43 Ang.
PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C13B - C18B .. 1.74 Ang.
PLAT361_ALERT_2_C Long C(sp3)-C(sp3) Bond C13D - C18D .. 1.67 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 112 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 18 Note
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 6 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for F5DA --C3D . 6.1 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for F7C --C6C . 14.1 s.u.

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PLAT230_ALERT_2_G Hirshfeld Test Diff for    F8CA     --C6C      .       13.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F9A      --C6A      .        7.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    F9AA     --C6A      .       18.4 s.u.
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C3C Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C3D Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C6A Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C6B Check
PLAT242_ALERT_2_G Low    'MainMol' Ueq as Compared to Neighbors of        C6D Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4DA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5DA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7DA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9DA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F4CA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F5CA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7CA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8CA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9A        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9C        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9D        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9CA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F7AA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8AA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F9AA       Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of F8DA       Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1  )         17% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )       100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  1        115.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  2          0.50 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for       C13B Check
PLAT344_ALERT_2_G Unusual sp?       Angle Range in Solvent/Ion for       C17B Check
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O14D          104.8 Degree
PLAT398_ALERT_2_G Deviating  C-O-C    Angle From 120 for O16C          109.7 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact  F8DA     ..C6D             1.73 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F8DA     ..C3D             2.19 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F8DA     ..C2D             2.95 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O14B     ..C17B            2.67 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O16B     ..C17B            1.78 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C12B     ..C17B            2.72 Ang.
                                                     x,y,z  =      1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  C13B     ..C17B            2.15 Ang.
                                                     x,y,z  =      1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         16 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C13B     --C18B          1.74 Ang.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        163 Check
             C13B -C18B -O16B    1.555   1.555   1.555            35.30 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        266 Check
             C6A  -F9AA -C3A     1.555   1.555   1.555            44.90 Deg.
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PLAT793_ALERT_4_G Model has Chirality at C13A       (Centro SPGR)          R Verify
PLAT793_ALERT_4_G Model has Chirality at C13B       (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at C13D       (Centro SPGR)          R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Dy       (III)     .       3.17 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        16 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        89% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        20 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         1 Note
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  0 ALERT level A = Most likely a serious problem - resolve or explain
 10 ALERT level B = A potentially serious problem, consider carefully
 39 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 68 ALERT level G = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 51 ALERT type 2 Indicator that the structure model may be wrong or deficient
 16 ALERT type 3 Indicator that the structure quality may be low
 47 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 07/08/2019; check.def file version of 30/07/2019

Datablock 252 - ellipsoid plot