checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FPR841X1

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: FPR841X1

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Bond precision:   C-C = 0.0074 A           Wavelength=0.71073

Cell:           a=15.8351(14)    b=23.865(2)          c=19.0098(19)
                alpha=90         beta=101.191(4)      gamma=90
Temperature:    150 K

                  Calculated                 Reported
Volume            7047.3(11)                 7047.4(11)
Space group       P 21/c                     P 21/c
Hall group        -P 2ybc                    -P 2ybc
Moiety formula    C51 H45 Dy F18 O10 S4,     C63 H73 Dy F18 O10 S4
                  2(C6 H14)
Sum formula       C63 H73 Dy F18 O10 S4      C63 H73 Dy F18 O10 S4
Mr                1622.96                    1622.95
Dx,g cm-3         1.530                      1.530
Z                 4                          4
Mu (mm-1)         1.280                      1.280
F000              3292.0                     3292.0
F000'             3295.37
h,k,lmax          20,30,24                   20,30,24
Nref              16176                      16127
Tmin,Tmax         0.732,0.825                0.684,0.825
Tmin'             0.657

Correction method= # Reported T Limits: Tmin=0.684 Tmax=0.825
AbsCorr = MULTI-SCAN

Data completeness= 0.997         Theta(max)= 27.484

R(reflections)= 0.0436( 12302)     wR2(reflections)= 0.1141( 16127)

S = 0.967                 Npar= 813
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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
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   23 Note

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Alert level C
PLAT213_ALERT_2_C Atom F2   has ADP max/min Ratio .....   3.6 prolat
PLAT213_ALERT_2_C Atom F3   has ADP max/min Ratio .....   3.4 prolat
PLAT213_ALERT_2_C Atom F9   has ADP max/min Ratio .....   3.7 prolat
PLAT213_ALERT_2_C Atom C17   has ADP max/min Ratio .....   3.1 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C   Ueq(max)/Ueq(min) Range   5.6 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H   Uiso(max)/Uiso(min) Range   7.2 Ratio
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C32 Check
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C57   - C58   .   1.42 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C58   - C59   .   1.41 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C59   - C60   .   1.41 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C60   - C61   .   1.37 Ang.
PLAT360_ALERT_2_C Short   C(sp3)-C(sp3) Bond C61   - C62   .   1.42 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H59A   ..H60A   1.98 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. #   1 Note
              C51 H45 Dy F18 O10 S4
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   2 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.24A   From C33   1.52 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H61A   -0.40 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

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Alert level G
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite   12 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension   1 Info
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings   Differ Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large   23.63 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records   2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records   4 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records   2 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records   4 Report
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C36 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C40 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C41 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C45 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C46 Check
PLAT242_ALERT_2_G Low   'MainMol' Ueq as Compared to Neighbors of   C50 Check
PLAT344_ALERT_2_G Unusual sp3   Angle Range in Solvent/Ion for   C60 Check
PLAT344_ALERT_2_G Unusual sp3   Angle Range in Solvent/Ion for   C61 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ....   1 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ....   42 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600   26 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....   2 Note

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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
  18 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  20 **ALERT level G** = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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25 ALERT type 2 Indicator that the structure model may be wrong or deficient
 5 ALERT type 3 Indicator that the structure quality may be low
 7 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 30/01/2018; check.def file version of 30/01/2018

NOMOVE FORCED
Prob = 50
Temp = 150

28 Y

PLATON-Feb 16 15:10:19 2018 - (70316)

Z -1   FPR841X1 P 21/c   R = 0.04   RES= 0   -1 X