checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_2418

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: exp_2418

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Bond precision:  C-C = 0.0067 A          Wavelength=1.54184

Cell:            a=16.7542(2)    b=14.7179(2)       c=22.3108(3)
                 alpha=90        beta=97.145(1)     gamma=90
Temperature:     100 K
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	Calculated	Reported
Volume	5458.82(12)	5458.82(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C24 B F20, C32 H58 B Dy P	C32 H58 B Dy P, B C24 F20
Sum formula	C56 H58 B2 Dy F20 P	C56 H58 B2 Dy F20 P
Mr	1326.11	1326.11
Dx,g cm-3	1.614	1.614
Z	4	4
Mu (mm-1)	8.551	8.551
F000	2660.0	2660.0
F000’	2631.95	
h,k,lmax	20,18,27	20,17,27
Nref	10587	10342
Tmin,Tmax	0.629,0.652	0.605,1.000
Tmin’	0.405	

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Correction method= # Reported T Limits: Tmin=0.605 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.977          Theta(max)= 71.219

R(reflections)= 0.0479( 9152)     wR2(reflections)= 0.1289( 10342)

S = 1.039                 Npar= 757
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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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PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.41 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  F   Ueq(max)/Ueq(min) Range       3.1 Ratio
PLAT356_ALERT_3_C Short   X-BH3      Distance  B1       - H1B           1.03 Ang.
PLAT356_ALERT_3_C Short   X-BH3      Distance  B1       - H1C           1.03 Ang.
PLAT357_ALERT_3_C Long    X-BH3      Distance  B1       - H1A           1.28 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        19 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  0.93A   From C4            1.67 eA-3
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Alert level G

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PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       7.72 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1      --P1       .       16.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1      --C4       .        9.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1      --C5       .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1      --C21      .        7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1A     --C1       .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1A     --C2       .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1A     --C3       .        6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1A     --C22      .        6.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Dy1A     --C23      .        5.3 s.u.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )         3% Note
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C1       - C6       .       1.53 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C2       - C9       .       1.52 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C3       - C12      .       1.53 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C5       - C18      .       1.51 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C21      - C25      .       1.52 Ang.
PLAT367_ALERT_2_G Long?  C(sp?)-C(sp?) Bond  C24      - C31      .       1.51 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact F3       ..F9               2.80 Ang.
                                              1-x,-y,1-z  =      3_656 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #         238 Check
             C4   -C15  -DY1A    1.555   1.555   1.555             43.70 Deg.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          2 Note
             C32 H58 B Dy P
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).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        218 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 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
  7 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 26 ALERT level G = General information/check it is not something unexpected

  2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 21 ALERT type 2 Indicator that the structure model may be wrong or deficient
  6 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  0 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 18/09/2020; check.def file version of 20/08/2020

Datablock exp_2418 - ellipsoid plot