checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 4

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: 4

Bond precision: C-C = 0.0121 A   Wavelength=0.71073

Cell: a=35.8608(10)   b=43.6134(13)   c=26.6974(7)
                 alpha=90   beta=96.885(3)   gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	41454(2)	41454(2)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C72 H60 Cl2 Dy O4 P4, Cl [+ solvent]	?
Sum formula	C72 H60 Cl3 Dy O4 P4 [+ solvent]	C72 H60 Cl3 Dy O4 P4
Mr	1381.93	1381.93
Dx,g cm-3	1.107	1.107
Z	20	20
Mu (mm-1)	1.113	1.113
F000	14020.0	14020.0
F000'	14037.40	
h,k,lmax	44,53,32	44,53,32
Nref	40736	40661
Tmin,Tmax	0.677,0.800	0.674,0.799
Tmin'	0.568	

Correction method= # Reported T Limits: Tmin=0.674 Tmax=0.799
AbsCorr = ANALYTICAL

Data completeness= 0.998   Theta(max)= 26.000

R(reflections)= 0.0640(27425)   wR2(reflections)= 0.1776(40661)

S = 1.022   Npar= 1915

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.

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🟠 **Alert level B**
DIFMN02_ALERT_2_B The minimum difference density is < -0.1*ZMAX*1.00
            _refine_diff_density_min given =   -6.606
            Test value =   -6.600
PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).   20 Note
PLAT973_ALERT_2_B Check Calcd Positive Resid. Density on   Dy2   1.71 eA-3

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🟡 **Alert level C**
DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
            The relevant atom site should be identified.
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
            The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density   5.51 eA-3
PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density   -6.61 eA-3
PLAT213_ALERT_2_C Atom C169   has ADP max/min Ratio .....   3.3 prolat
PLAT213_ALERT_2_C Atom Cl19   has ADP max/min Ratio .....   3.1 prolat
PLAT213_ALERT_2_C Atom C151   has ADP max/min Ratio .....   3.2 prolat
PLAT213_ALERT_2_C Atom C154   has ADP max/min Ratio .....   3.8 prolat
PLAT213_ALERT_2_C Atom C178   has ADP max/min Ratio .....   3.5 prolat
PLAT213_ALERT_2_C Atom C180   has ADP max/min Ratio .....   3.1 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 3 C   Ueq(max)/Ueq(min) Range   3.3 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for   P16   --O8   .   6.3 s.u.
PLAT234_ALERT_4_C Large Hirshfeld Difference C138   --C155   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C103   --C128   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C129   --C165   0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C135   --C141   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C148   --C164   0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C157   --C171   0.17 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C169 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C133 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   O13 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C154 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C166 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C176 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C178 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of   C180 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C19 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C72 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C90 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C93 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C125 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C137 Check
PLAT242_ALERT_2_C Low   'MainMol' Ueq as Compared to Neighbors of   C161 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....   2.3 Note
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C90   -C154   1.37 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C93   -C132   1.36 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C103   -C149   1.37 Ang.
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist C125   -C160   1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.01207 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...   -3.279 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=   0.600   33 Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on   Dy1   1.24 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.   0 Info

Alert level G

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PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical          ? Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT   Unusually Large    538.92 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy3        --O8        .      5.7 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4         Constrained at      0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5         Constrained at      0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )     100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  8  )     100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ...... Resd  4        0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  5         0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  6         0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  7         0.50 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in ..... Resd  8         0.50 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure     ! Info
PLAT794_ALERT_5_G Tentative Bond Valency for Dy1        (III)    .     3.27 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Dy2        (III)    .     3.20 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Dy3        (III)    .     3.23 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed        ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      22 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       9 Note
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
  44 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

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  38 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
  24 ALERT type 4 Improvement, methodology, query or suggestion
   3 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 23/04/2018; check.def file version of 23/04/2018