checkCIF/PLATON report

Structure factors have been supplied for datablock(s) a_sq

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: a_sq

Bond precision: C-C = 0.0199 A   Wavelength=0.71073

Cell: a=14.0526(14)   b=14.0526(14)   c=46.815(5)
                   alpha=90   beta=90   gamma=90
Temperature: 120 K

	Calculated	Reported
Volume	9245(2)	9245(2)
Space group	P 43	P 43
Hall group	P 4cw	P 4cw
Moiety formula	2(C46 H39 Dy N10 O4), 3(H2 O) [+ solvent]	C46 H39 Dy N10 O4, 1.5(H2 O)
Sum formula	C92 H84 Dy2 N20 O11 [+ solvent]	C46 H42 Dy N10 O5.50
Mr	1970.79	985.39
Dx,g cm-3	1.416	1.416
Z	4	8
Mu (mm-1)	1.673	1.673
F000	3984.0	3984.0
F000'	3983.80	
h,k,lmax	18,18,61	18,18,61
Nref	22365[11318]	21755
Tmin,Tmax	0.685,0.706	0.598,0.746
Tmin'	0.672	

Correction method= # Reported T Limits: Tmin=0.598 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.92/0.97   Theta(max)= 28.000

R(reflections)= 0.0625(15345)   wR2(reflections)= 0.1397(21755)

S = 0.992   Npar= 1123

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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PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) .......      9 Report
              C2A'    C2      C3A'    C3      C4A'    C4            etc.
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Author Response: Due to severe disorder on the ligands some atoms were refined isotropically.

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PLAT420_ALERT_2_B D-H Without Acceptor      O2W     --H2WB    .    Please Check
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Author Response: This is because the SQUEEZE procedure has been applied.

🟡 Alert level C

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PLAT220_ALERT_2_C NonSolvent Resd 1  C   Ueq(max) / Ueq(min) Range      3.9 Ratio
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of      C19 Check
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of      C19A Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C17      --C22      .      1.37 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............  0.01992 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600       3 Report
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Dy1    1.07 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on      Dy2    1.02 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  1.09A   From N4A      0.54 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H3WA      -0.32 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H23E      -0.35 eA-3
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⚪ Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite      24 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       8 Report
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .   0.215 Note
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ   Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...   0.50 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records       8 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       4 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )     10% Note
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  2 )      5% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C23 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....   C23A Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H2     ..H14C    .      2.09 Ang.
                                             x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H4     ..H23A    .      1.98 Ang.
                                             x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H23A   ..H4'     .      1.93 Ang.
                                             x,y,z =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn      H14I   ..H2B'    .      1.89 Ang.
                                             x,y,z =      1_555 Check
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure     ! Info
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      19 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      21 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed       ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       2 Note
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PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....       1 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...       8 Note
PLAT960_ALERT_3_G Number of Intensities with I  <   - 2*sig(I) ...       4 Check
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
   2 ALERT level B = A potentially serious problem, consider carefully
  11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  25 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  18 ALERT type 2 Indicator that the structure model may be wrong or deficient
   8 ALERT type 3 Indicator that the structure quality may be low
   9 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 22/12/2019; check.def file version of 13/12/2019

NOMOVE FORCED

Prob = 50
Temp = 120

50 Y

PLATON-Apr 15 13:55:39 2020 - (70316)

Z -81   a_sq   P 43   R = 0.06   RES=   0   97 X