checkCIF/PLATON report

Structure factors have been supplied for datablock(s) hol2

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: hol2

Bond precision: C-C = 0.0094 A Wavelength=0.79272

Cell: a=20.115(4) b=19.538(2) c=25.698(5)
alpha=90 beta=104.258(16) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	9788(3)	9788(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C46 H39 Ho N10 O4, C H2 Cl2, C H4 O [+ solvent]	C46 H39 Ho N10 O4, C H2 Cl2, C H4 O [+ SOLVENT]
Sum formula	C48 H45 Cl2 Ho N10 O5 [+ solvent]	C48 H45 Cl2 Ho N10 O5
Mr	1077.77	1077.77
Dx,g cm-3	1.463	1.463
Z	8	8
Mu (mm-1)	2.362	2.375
F000	4352.0	4352.0
F000’	4354.87	
h,k,lmax	24,23,30	24,23,30
Nref	17894	17880
Tmin,Tmax	0.752,0.827	0.001,1.000
Tmin’	0.652	

Correction method= # Reported T Limits: Tmin=0.001 Tmax=1.000
AbsCorr = EMPIRICAL

Data completeness= 0.999 Theta(max)= 28.500

R(reflections)= 0.0528(13358) wR2(reflections)= 0.1601(17880)

S = 1.270 Npar= 1206

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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PLAT220_ALERT_2_C NonSolvent Resd 2  C   Ueq(max) / Ueq(min) Range        3.2 Ratio
PLAT241_ALERT_2_C High   MainMol Ueq as Compared to Neighbors of       C11A Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of        C3S Check
PLAT244_ALERT_4_C Low    Solvent Ueq as Compared to Neighbors of        C4S Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl1      0.153 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cl3      0.159 Check
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.00944 Ang.
PLAT414_ALERT_2_C Short Intra D-H..H-X       H5       ..H23H            1.92 Ang.
                                                      x,y,z  =      1_555 Check
PLAT420_ALERT_2_C D-H Without Acceptor       N5       --H5       .     Please Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.345 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         14 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density.          0 Info
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Alert level G

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ABSMU01_ALERT_1_G  Calculation of _exptl_absorpt_correction_mu
                not performed for this radiation type.
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          7 Note
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          3 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       9.41 Why ?
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    0.79272 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          4 Report
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure        101 A**3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........         11 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         4 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed           ! Info
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        56% Note
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 ...        13 Note
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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
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  10 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
   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 22/12/2019; check.def file version of 13/12/2019

Datablock hol2 - ellipsoid plot