checkCIF/PLATON report

Structure factors have been supplied for datablock(s) d1789a_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: d1789a_a_sq

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Bond precision:  C-C = 0.0148 A          Wavelength=0.71073

Cell:           a=17.0922(15)    b=22.4119(17)     c=15.7288(14)
                alpha=90         beta=92.427(3)    gamma=90
Temperature:    150 K
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	Calculated	Reported
Volume	6019.8(9)	6019.8(9)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C69 H42 Ho N9 O3 [+ solvent]	C69 H42 Ho N9 O3
Sum formula	C69 H42 Ho N9 O3 [+ solvent]	C69 H42 Ho N9 O3
Mr	1210.05	1210.04
Dx,g cm-3	1.335	1.335
Z	4	4
Mu (mm-1)	1.368	1.368
F000	2440.0	2440.0
F000’	2439.89	
h,k,lmax	22,29,20	22,29,20
Nref	6973	6963
Tmin,Tmax	0.821,0.872	0.631,0.746
Tmin’	0.740	

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Correction method= # Reported T Limits: Tmin=0.631 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.999          Theta(max)= 27.549

R(reflections)= 0.1087( 5145)     wR2(reflections)= 0.2178( 6963)

S = 1.370                 Npar= 492
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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

PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT215_ALERT_3_C Disordered C7A has ADP max/min Ratio ..... 3.1 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 3.0 Note
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01484 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 17.484 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 5.158 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.558 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 1 Check
PLAT977_ALERT_2_C Check the Negative Difference Density on H18A -0.41 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 55 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 27 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 117.98 Why ?
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 1 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 3 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Ho1 -- N3 .. 6.5 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O1A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N1A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N2A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N3A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C1A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C5A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C6A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C8A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C9A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C10A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C11A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C12A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C13A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C14A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C15A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C16A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C22A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C23A is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3AA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4AA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H5AA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H6AA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H9AA is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H10B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H11B is Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H12B is Constrained at 0.5 Check

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PLAT300_ALERT_4_G Atom Site Occupancy of H16B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H17B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H18A    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H20B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H21B    is Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H22B    is Constrained at        0.5 Check
PLAT301_ALERT_3_G Main Residue  Disorder .............(Resd  1)..         33 % Note
PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C1     -C14          1.44 Ang.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure       156 A**3
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Author Response: During the refinement of the structure, electron density peaks were located that were believed to be highly disordered solvent molecules (possibly CHCl2/CH3CN). Attempts made to model the solvent molecule were not successful. The SQUEEZE option in PLATON (Spek, 2009) indicated there was a large solvent cavity of 156A3 . In the final cycles of refinement, this contribution of 65 electrons to the electron density was removed from the observed data. The density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option PLATON (Spek, 2009). Similar treatments of disordered solvent molecules were carried out by St\"ahler et al. (2001), Cox et al. (2003), Mohamed et al. (2003) and Athimoolam et al. (2005). References: Spek, A. L. (2009). *Acta Cryst.* D65, 148--155. Athimoolam, S., Kumar, J., Ramakrishnan, V. & Rajaram, R.K. (2005). Acta Cryst. E61, m2014-m2017. Cox, J.P., Kumarasammy, Y., Nahar, L., Sarkar D.S. & Shoeb, M. (2003). Acta Cryst. E59, o975-o977. Mohamed, A.A., Krause Bauer, A.J., Bruce, E.A. & Bruce M.R.M. (2003). Acta Cryst. C59, m84-m86. St\"ahler, R., N\"ather, C. & Bensch, W. (2001). Acta Cryst. C57, 26-27.**

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          5 Note
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group  #        41 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....         ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       306 Note
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        10 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         4 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
  10 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  58 ALERT level G = General information/check it is not something unexpected

   0 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
   8 ALERT type 3 Indicator that the structure quality may be low
  49 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 27/03/2017; check.def file version of 24/03/2017

Datablock d1789a_a_sq - ellipsoid plot