checkCIF/PLATON report

Structure factors have been supplied for datablock(s) phb157r

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: phb157r

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Bond precision:  C-C = 0.0061 A          Wavelength=0.71073

Cell:            a=7.3486(3)     b=31.9323(13)     c=10.1572(4)
                 alpha=90        beta=90           gamma=90
Temperature:     296 K
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	Calculated	Reported
Volume	2383.47(17)	2383.47(17)
Space group	P n m a	P n m a
Hall group	-P 2ac 2n	-P 2ac 2n
Moiety formula	C18 H22 Ba N4 O12	C18 H22 Ba N4 O12
Sum formula	C18 H22 Ba N4 O12	C18 H22 Ba N4 O12
Mr	623.73	623.73
Dx,g cm-3	1.738	1.738
Z	4	4
Mu (mm-1)	1.735	1.735
F000	1240.0	1240.0
F000’	1239.37	
h,k,lmax	8,37,12	8,37,12
Nref	2134	2130
Tmin,Tmax	0.812,0.917	0.637,0.745
Tmin’	0.771	

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Correction method= # Reported T Limits: Tmin=0.637 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 25.000

R(reflections)= 0.0314( 1801)     wR2(reflections)= 0.0712( 2130)

S = 1.095                 Npar= 175
```

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

PLAT975_ALERT_2_B Check Calcd Resid. Dens. 0.99A From O7 1.67 eA-3

Author Response: The electron density peak is near to O7. By visual inspection of ellipsoid of O7, it is found that there is no disorder for O7. No other atom can be accounted for in this position. Since the crystal is a coordination polymer, this may be due to poor absorption correction in a heavy atom (Ba) structure.

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.08 Report
PLAT213_ALERT_2_C Atom O1 has ADP max/min Ratio ..... 3.3 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 4.7 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O5 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Ba1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.6 Note
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.99A From O7 1.67 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety ..... C9 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.17 Ratio
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Ba1 --Ba1 .. 4.25 Ang.
PLAT774_ALERT_1_G Suspect X-Y Bond in CIF: Ba1 --Ba1 .. 4.25 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 3 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still 71% Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 4 Note
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
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
11 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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 17/03/2019; check.def file version of 04/03/2019

Datablock phb157r - ellipsoid plot