

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 2

Bond precision:	Br-Br = 0.0060 Å	Wavelength=0.71073	
Cell:	a=13.0997(11)	b=13.6459(13)	c=27.906(3)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	4988.4(8)	4988.4(8)	
Space group	P b a m	Pbam	
Hall group	-P 2 2ab	?	
Moiety formula	Br36 Dy6 Hg9	Br36 Dy6 Hg9	
Sum formula	Br36 Dy6 Hg9	Br36 Dy6 Hg9	
Mr	5656.71	5656.71	
Dx, g cm-3	3.766	3.741	
Z	2	2	
Mu (mm-1)	32.644	31.850	
F000	4752.0	4722.0	
F000'	4700.90		
h, k, lmax	15, 16, 33	15, 16, 33	
Nref	4514	4402	
Tmin, Tmax	0.090, 0.148	0.090, 0.148	
Tmin'	0.068		

Correction method= # Reported T Limits: Tmin=0.090 Tmax=0.148
AbsCorr = MULTI-SCAN

Data completeness= 0.975 Theta(max)= 25.030

R(reflections)= 0.1122(2666) wR2(reflections)= 0.3482(4402)

S = 1.032 Npar= 125

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 A

PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure

! Info

Alert level B

PLAT241_ALERT_2_B	High	'MainMol' Ueq as Compared to Neighbors of	Hg1	Check
PLAT241_ALERT_2_B	High	'MainMol' Ueq as Compared to Neighbors of	Hg2	Check
PLAT242_ALERT_2_B	Low	'MainMol' Ueq as Compared to Neighbors of	Br8	Check

Alert level C

ABSMU01_ALERT_1_C The ratio of given/expected absorption coefficient lies outside the range 0.99 <> 1.01
Calculated value of mu = 32.644
Value of mu given = 31.850

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75
_refine_diff_density_min given = -6.423
Test value = -6.000

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full	value Low	0.975	Why?
PLAT051_ALERT_1_C	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by		2.49	%
PLAT068_ALERT_1_C	Reported F000 Differs from Calcd (or Missing)...			Please Check
PLAT082_ALERT_2_C	High R1 Value		0.11	Report
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25)		0.35	Report
PLAT098_ALERT_2_C	Large Reported Min. (Negative) Residual Density		-6.42	eA-3
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		Hg3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Dy3	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Br5	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	Hg1	0.104	Check

Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF		Please Do !
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large	0.19	Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	179.14	Why ?
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature (K)	293	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Hg1 (II)	2.19	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Hg3 (II)	2.07	Info
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON	85	Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
3 **ALERT level B** = A potentially serious problem, consider carefully
13 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

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

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT602_2
;
PROBLEM: VERY LARGE Solvent Accessible VOID(S) in Structure      ! Info
RESPONSE: ...
;
_vrf_PLAT241_2
;
PROBLEM: High      'MainMol' Ueq as Compared to Neighbors of      Hg1 Check
RESPONSE: ...
;
_vrf_PLAT242_2
;
PROBLEM: Low      'MainMol' Ueq as Compared to Neighbors of      Br8 Check
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 03/05/2019; check.def file version of 29/04/2019

