

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: c__dycomp~1__dyop~2_p21c

Bond precision:	C-C = 0.0043 A	Wavelength=0.71073	
Cell:	a=19.684(4)	b=15.211(3)	c=34.082(7)
	alpha=90	beta=95.91(3)	gamma=90
Temperature:	123 K		
	Calculated	Reported	
Volume	10150(4)	10150(3)	
Space group	P 21/c	P2(1)/c	
Hall group	-P 2ybc	?	
Moiety formula	2(C54 H45 Cl3 Dy O3 P3), C3 H6 O	?	
Sum formula	C111 H96 Cl6 Dy2 O7 P6	C55.50 H48 Cl3 Dy O3.50 P3	
Mr	2265.40	1132.70	
Dx,g cm-3	1.482	1.482	
Z	4	8	
Mu (mm-1)	1.769	1.769	
F000	4568.0	4568.0	
F000'	4573.81		
h,k,lmax	25,20,44	25,19,44	
Nref	24284	24163	
Tmin,Tmax	0.432,0.702	0.432,0.702	
Tmin'	0.409		

Correction method= # Reported T Limits: Tmin=0.432 Tmax=0.702

AbsCorr = MULTI-SCAN

Data completeness= 0.995 Theta(max)= 27.910

R(reflections)= 0.0322(23070) wR2(reflections)= 0.0826(24163)

S = 1.076 Npar= 1227

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

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C	Ueq(max)/Ueq(min) Range	4.3	Ratio
PLAT241_ALERT_2_C	High 'MainMol'	Ueq as Compared to Neighbors of	C39	Check
PLAT242_ALERT_2_C	Low 'MainMol'	Ueq as Compared to Neighbors of	C37	Check
PLAT242_ALERT_2_C	Low 'MainMol'	Ueq as Compared to Neighbors of	C40	Check
PLAT411_ALERT_2_C	Short Inter H...H Contact	H14 ..H86	2.10	Ang.

● Alert level G

PLAT005_ALERT_5_G	No Embedded Refinement Details Found	in the CIF	Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...		0.50 Check
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large	21.35 Why ?
PLAT093_ALERT_1_G	No s.u.'s on H-positions, Refinement Reported as		mixed Check
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dy1	--Cl1 .	5.5 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dy1	--Cl3 .	6.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dy2	--Cl4 .	8.3 s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dy2	--Cl6 .	7.3 s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O1'	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of ClS'	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S'	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C4'	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S4	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S5	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S6	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S4	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S5	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S6	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1S	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of ClS	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2S	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3S	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1S3	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S1	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S2	Constrained at	0.5 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2S3	Constrained at	0.5 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)		100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 4)		100% Note
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety		C2S Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels		14 Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy1 (III)		3.21 Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL		2018 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
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
35 **ALERT level G** = General information/check it is not something unexpected
- 3 **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
0 **ALERT type 3** Indicator that the structure quality may be low
25 **ALERT type 4** Improvement, methodology, query or suggestion
2 **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 30/01/2018; check.def file version of 30/01/2018

