

# checkCIF/PLATON report

Structure factors have been supplied for datablock(s) r

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: r

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Bond precision:    C-C = 0.0100 A

Wavelength=0.71073

Cell:                a=12.6856(12)        b=13.2662(13)        c=17.0051(16)  
                      alpha=84.098(2)      beta=74.746(2)      gamma=62.038(2)  
Temperature:        120 K

	Calculated	Reported
Volume	2437.9(4)	2437.9(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C100 H94 Dy2 N20 O16, 2(C2 H6 O), H2 O	C50 H47 Dy N10 O8, C2 H6 O, (H2 O)0.5
Sum formula	C104 H108 Dy2 N20 O19	C52 H54 Dy N10 O9.50
Mr	2267.11	1133.55
Dx, g cm-3	1.544	1.544
Z	1	2
Mu (mm-1)	1.603	1.603
F000	1156.0	1156.0
F000'	1156.05	
h,k,lmax	17,18,23	17,18,23
Nref	12944	12799
Tmin,Tmax	0.674,0.737	0.611,0.746
Tmin'	0.593	

Correction method= # Reported T Limits: Tmin=0.611 Tmax=0.746  
AbsCorr = MULTI-SCAN

Data completeness= 0.989

Theta(max)= 29.000

R(reflections)= 0.0578( 10484)

wR2(reflections)= 0.1571( 12799)

S = 1.122

Npar= 673

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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.

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### ● Alert level C

PLAT213_ALERT_2_C	Atom C14A	has ADP max/min Ratio	.....	3.4	prolat
PLAT220_ALERT_2_C	NonSolvent Resd 1	C	Ueq(max) / Ueq(min) Range	4.5	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range	4.2	Ratio
PLAT241_ALERT_2_C	High MainMol Ueq as Compared to Neighbors of				O1A Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	.....		0.00997	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		32	Report
PLAT918_ALERT_3_C	Reflection(s) with I(obs) much Smaller I(calc)	.		1	Check

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### ● Alert level G

PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	.....		6	Report
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor	...		0.50	Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)			0.002	Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Dy1	--O1	.	6.2	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of O4	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O4'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7A'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8A'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C7A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C8A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C9A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10"	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C10A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11"	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C11A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12"	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C12A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13"	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C13A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C18'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C19'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C20'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C21'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C22'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C25'	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3NA	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3B	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AA	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H9AB	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10B	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H10C	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12B	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H12C	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13B	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H13C	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18A	Constrained at		0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H18B	Constrained at		0.5	Check

PLAT300_ALERT_4_G	Atom Site Occupancy of H19A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H19B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H21B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22A	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H22B	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25D	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25E	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25F	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25G	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25H	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H25I	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 C1S	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 H1SO	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1SB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SC	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O2S	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 C4S	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3SA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3SB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SB	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H4SC	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2SD	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of O1W	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1WA	Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1WB	Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1 )		20%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2 )		100%	Note
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
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 2 )		4.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 3 )		4.50	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 4 )		1.50	Check
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C17 -C22		0.19	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C17 -C22'		0.19	Ang.
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O3A		18.7	Degree
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H18B ..H24F .		2.12	Ang.
	1-x,-y,2-z =		2_657	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X H3NA ..H14D		1.91	Ang.
	x,y,z =		1_555	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X H3B ..H13A		2.04	Ang.
	x,y,z =		1_555	Check
PLAT414_ALERT_2_G	Short Intra D-H..H-X H3B ..H14A		1.89	Ang.
	x,y,z =		1_555	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....		23	Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		2	Note
	C2 H6 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		3	Note
	C2 H6 O			
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #		4	Note
	H2 O			
PLAT804_ALERT_5_G	Number of ARU-Code Packing Problem(s) in PLATON		1	Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..		!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600		118	Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law ( 1 2 0 ) Est.d BASF		0.39	Check

PLAT933\_ALERT\_2\_G Number of OMIT Records in Embedded .res File ... 19 Note  
PLAT960\_ALERT\_3\_G Number of Intensities with  $I < - 2*\text{sig}(I)$  ... 4 Check

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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  
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
102 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
12 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  
85 ALERT type 4 Improvement, methodology, query or suggestion  
3 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.

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**PLATON version of 22/12/2019; check.def file version of 13/12/2019**

