

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 1

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: 1

Bond precision: C-C = 0.0065 A

Wavelength=0.71073

Cell: a=14.5732(17) b=15.9915(19) c=19.048(2)
 alpha=91.490(2) beta=91.613(2) gamma=112.743(2)
Temperature: 150 K

	Calculated	Reported
Volume	4089.0(8)	4089.1(8)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C63 H63 Dy N5 O2, C24 H20 B, 0.5(C8 H8), C7 H8	C63 H63 Dy N5 O2, C24 H20 B, C7 H8, C4 H4
Sum formula	C98 H95 B Dy N5 O2	C98 H95 B Dy N5 O2
Mr	1548.10	1548.09
Dx,g cm-3	1.257	1.257
Z	2	2
Mu (mm-1)	0.966	0.966
F000	1610.0	1610.0
F000'	1610.11	
h,k,lmax	17,19,22	17,19,22
Nref	14391	14309
Tmin,Tmax	0.840,0.857	0.673,0.745
Tmin'	0.840	

Correction method= # Reported T Limits: Tmin=0.673 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.994

Theta(max)= 24.999

R(reflections)= 0.0370(12006)

wR2(reflections)= 0.0907(14309)

S = 1.044

Npar= 979

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O1	--C39	.	5.5 s.u.
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Dy1	--O1	.	5.2 s.u.
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of				C63 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of				C94 Check
PLAT260_ALERT_3_C	Large Average Ueq of Residue Including		C96		0.195 Check
PLAT332_ALERT_2_C	Large Phenyl C-C Range	C78	-C87	.	0.19 Ang.
PLAT412_ALERT_2_C	Short Intra XH3 .. XHn	H96	..H99B	.	1.80 Ang.
			2-x,-y,1-z =		2_756 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.595			80 Report

● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite				4 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...				17 Report
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ				Please Check
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)				0.002 Degree
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records				1 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records				4 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records				1 Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records				5 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records				2 Report
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)				4% Note
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for				C97 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				1 Note
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C98		--C98		1.91 Ang.
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters				1 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints				77 Note
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still				75% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).				3 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				25 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity				2.6 Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				1 Info

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

2 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
 8 ALERT type 4 Improvement, methodology, query or suggestion
 0 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.

