

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: 1

Bond precision:	C-C = 0.0129 Å	Wavelength=0.71073
Cell:	a=19.0929(14)	b=26.7829(17) c=24.9829(18)
	alpha=90	beta=91.547(3) gamma=90
Temperature:	180 K	
	Calculated	Reported
Volume	12770.7(15)	12770.7(15)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C135 H85 Dy4 N O26 [+ solvent]	?
Sum formula	C135 H85 Dy4 N O26 [+ solvent]	C135 H95 Dy4 N O29
Mr	2787.05	2845.08
Dx, g cm ⁻³	1.450	1.478
Z	4	4
Mu (mm ⁻¹)	2.383	2.386
F000	5496.0	5616.0
F000'	5495.31	
h, k, lmax	24, 34, 32	24, 34, 32
Nref	29319	29233
Tmin, Tmax	0.570, 0.788	0.570, 0.788
Tmin'	0.381	

Correction method= # Reported T Limits: Tmin=0.570 Tmax=0.788

AbsCorr = EMPIRICAL

Data completeness= 0.997

Theta(max)= 27.494

R(reflections)= 0.0587(19905)

wR2(reflections)=
0.1664(29233)

S = 1.044

Npar= 1393

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

PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O2	--H2A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O3	--H3A	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O3	--H3B	.	Please Check
PLAT420_ALERT_2_B	D-H Bond Without Acceptor	O5	--H5A	.	Please Check



Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as empirical

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C76	--C90	.	5.5 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C77	--C82	.	5.7 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C81	--C82	.	6.0 s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C83	--C84	.	6.0 s.u.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C75	Check		
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds				0.01286 Ang.
PLAT415_ALERT_2_C	Short Inter D-H..H-X	H2A	..H10	.	2.06 Ang.
		1-x,1-y,-z	=		3_665 Check
PLAT415_ALERT_2_C	Short Inter D-H..H-X	H3B	..H10	.	2.03 Ang.
		1-x,1-y,-z	=		3_665 Check



Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.

Atom count from _chemical_formula_sum: C135 H95 Dy4 N1 O29

Atom count from the _atom_site data: C135 H85 Dy4 N1 O26

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests

From the CIF: _cell_formula_units_Z 4

From the CIF: _chemical_formula_sum C135 H95 Dy4 N O29

TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	540.00	540.00	0.00
H	380.00	340.00	40.00
Dy	16.00	16.00	0.00
N	4.00	4.00	0.00
O	116.00	104.00	12.00

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	6	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	137	Report
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	4	Report
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ		Please Check

PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical		? Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	62.76	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	4	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	5	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	3	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	3	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200	Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0100	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT192_ALERT_3_G	A Non-default DELU Restraint Value for First Par	0.0010	Report
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C2 -C7	0.17	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C9 -C14	0.20	Ang.
PLAT335_ALERT_2_G	Check Large C6 Ring C-C Range C24 -C29	0.15	Ang.
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure		! Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy1 (III) .	2.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy2 (III) .	2.97	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy3 (III) .	3.04	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Dy4 (III) .	2.87	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	3607	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed		! Info
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .		Please Do !
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.6	Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged		Please Check

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

6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 19 ALERT type 2 Indicator that the structure model may be wrong or deficient
 9 ALERT type 3 Indicator that the structure quality may be low
 7 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.

