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: FM108B

```
Bond precision:  C-C = 0.0068 A          Wavelength=0.71073

Cell:          a=8.2231(11)      b=12.833(2)      c=17.175(2)
               alpha=80.864(7)   beta=77.901(7)   gamma=88.862(8)
Temperature:   273 K
```

	Calculated	Reported
Volume	1749.5(4)	1749.5(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C64 H70 Dy2 O22 S2	C32 H35 Dy O11 S
Sum formula	C64 H70 Dy2 O22 S2	C32 H35 Dy O11 S
Mr	1580.32	790.16
Dx,g cm-3	1.500	1.500
Z	1	2
Mu (mm-1)	2.250	2.250
F000	794.0	794.0
F000’	794.24	
h,k,lmax	10,16,21	10,16,21
Nref	7156	7081
Tmin,Tmax	0.763,0.835	
Tmin’	0.746	

```
Correction method= Not given

Data completeness= 0.990          Theta(max)= 26.371

R(reflections)= 0.0354( 5879)     wR2(reflections)= 0.0816( 7081)

S = 1.048                 Npar= 419
```

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

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C31 Check
PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C32 Check

---

Alert level C

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.33 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.9 Ratio
PLAT222_ALERT_3_C Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range 5.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference S1A --C32 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference S1B --C31 0.19 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C6 Check
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 77 Ang**3

Alert level G

PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT012_ALERT_1_G No _shelx_res_checksum Found in CIF ..... Please Check
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
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 273 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 273 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy1 --O5 . 5.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Dy1 --O8_a . 5.6 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of S1A Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of S1B Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31A Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31B Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31C Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32A Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32C Constrained at 0.8 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31D Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31E Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H31F Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32D Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32E Constrained at 0.2 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32F Constrained at 0.2 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 2% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 19 Note

---

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

5 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
2 ALERT type 3 Indicator that the structure quality may be low
16 ALERT type 4 Improvement, methodology, query or suggestion
1 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

Datablock FM108B - ellipsoid plot